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STATISTICAL MODELING OF THERMAL-RADIATION TRANSFER IN NATURAL-CONVECTION TURBULENT DIFFUSION FLAMES. 1. MODEL CONSTRUCTION

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Methods of calculation of radiation transfer, which are used in modeling turbulent diffusion flames, are analyzed. Realization of the statistical method (Monte Carlo method) in combination with the equations of turbulent flow and combustion of a multicomponent mixture which is formed in combustion of hydrocarbons in air is presented. A method of calculation of the effective coefficient of absorption for a mixture of absorbing gases and soot is described. The effect of turbulent temperature fluctuations on the emission of thermal radiation is taken into account.

Introduction. Natural-convection turbulent diffusion flames are formed in fires. The adequacy of modeling of this phenomenon is to a great extent determined by calculation of thermal-radiation transfer. The model of radiation transfer must, first of all, correctly describe radiation heat transfer inside the flame and in the flow of combustion products, since this determines the structure and dynamics of the flame. Moreover, engineering practice requires calculation of radiation heat fluxes emitted by the flame and incident on the surrounding surfaces. This is essential in modeling of the ignition and combustion of solid and liquid fuels in order to determine the rate of warming-up, gasification, and thermal degradation of material, delay-time of ignition, and the velocity of propagation of the flame. At the same time, calculation of thermal-radiation transfer in combustion processes is a complex problem [1].

In modeling of flames, use is traditionally made of the following methods of calculation of thermal-radiation transfer: the methods of flow and moments [1, 2], the spherical harmonics method [3, 4], the discrete transfer method [5], the finite volume method, [6], and the discrete ordinate method [7]. All of the above methods, except for the spherical-harmonics method, which is also called the diffusion method, are intended for the approximate solution of the equation of radiation transfer along a fixed set of directions in space, which correspond to a set of segments into which the whole solid angle is split.

The presence of the fixed spatial directions along which radiation is transferred leads to the fact that the results of the calculation are very sensitive to their quantity. The error of digitization of the solid angle (beam effect) becomes particularly appreciable in the case where calculation of the heat flux emitted by a local source and incident on a remote surface is required (see, e.g., [8, 9]). An increase in the number of directions of radiation transfer can fail from the computational viewpoint, since it is rather difficult to adapt their selection to the problem under consideration, especially in an unsteady process.

The diffusion method presupposes the isotropic distribution of radiation intensity over the solid angle, which results in an elliptic equation for the radiation-energy density. However, the assumption of the angular isotropy of the radiation intensity restricts the use of the diffusion method, which, in particular, can lead to appreciable errors in calculation of flows incident on remote surfaces if the considered medium is strongly nonuniform (e.g., if the radiation source is surrounded by translucent air). Moreover, the elliptic equations of the diffusion method involve the coefficient of diffusion, which is in inverse proportion to the coefficient of absorption. In the above-noted case of the strong nonuniformity of the medium, the coefficient of diffusion changes in space by several orders of magnitude and has large gradients on interfaces. This noticeably deteriorates the convergence of numerical methods which have been developed for fast solution of elliptic equations with smooth coefficients of diffusion.

The employment of the statistical approach (see [4, 10] and others) is a natural way to overcome the above difficulties. This approach does not employ splitting of the solid angle and is not aimed at solving the equation of ra-

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diation transfer — it implements the idea underlying the derivation of this equation. Because of the random and constantly changing selection of the directions of radiation transfer, none of the spatial directions is given preference. The statistical method can pliably be adapted to this type of problem; therefore, in calculations of radiation heat transfer, it is often used as the standard method. We note that it was successfully used in modeling of fireballs [11, 12]; however, it is assumed to be expensive and is least often used in modeling of combustion.

This series of works is aimed at demonstrating the advantages and computational efficiency of the statistical method (Monte Carlo method) of calculation of radiation transfer in modeling of the combustion in flames of hydrocarbon fuels in air. In what follows, we give a description of the statistical method simultaneously with the models of turbulence, combustion, and radiation properties of radiating gases and soot. An algorithm of approximate account for the effect of turbulent fluctuations on the emission of thermal radiation is presented.

Modeling of Turbulence and Combustion. The suggested model is based on the system of Navier–Stokes equations of a multicomponent compressible reacting gas, which is averaged according to Favre [13]. The continuity equations, the equations of component transfer, and the equations of motion and energy have the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 , \tag{1}$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_j Y_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Sc}} + \frac{\mu_{\text{ò}}}{\mathrm{Sc}_{\text{ò}}}\right)\frac{\partial Y_\alpha}{\partial x_j} + \rho \dot{R}_\alpha , \tag{2}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i , \quad i = 1, 2, 3 , \tag{3}$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Pr}} + \frac{\mu_{\mathrm{t}}}{\mathrm{Pr}_{\mathrm{t}}}\right)\frac{\partial h}{\partial x_j} + \frac{\partial q_j^{\mathrm{r}}}{\partial x_j} , \tag{4}$$

where

$$\tau_{ij} = (\mu + \mu_{\mathrm{t}})\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\,\delta_{ij}\left(\rho k + (\mu + \mu_{\mathrm{t}})\,\frac{\partial u_k}{\partial x_k}\right);$$

$$h = \sum_{\alpha} Y_\alpha \left(\Delta h^0_{\mathrm{f}\alpha} + \int_{T^0}^{T} C_{P\alpha}(T)\, dT\right).$$

We considered a multicomponent mixture of gases (fuel, O_2, CO_2, H_2O, N_2, CO) and soot (C). The dependence of the isobaric heat capacity of the components on the temperature was approximated by polynomials of second order. For the considered substantially subsonic flow, the density of the gas mixture was determined from the equation of state

$$P = R\rho T \sum_{\alpha \neq \mathrm{C}} \frac{Y_\alpha}{M_\alpha} , \tag{5}$$

where the total pressure P was assumed to be equal to atmospheric pressure. To close the system of averaged equations we used the k–ε model. In the equations of transfer of the turbulence kinetic energy k and the rate of its dissipation ε

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_\mathrm{t}}{\sigma_k}\right)\frac{\partial k}{\partial x_j} + \rho\,(G + G_\mathrm{B}) - \rho\varepsilon\,, \tag{6}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho u_j \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_\mathrm{t}}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j} + \rho\,(C_{\varepsilon 1}\,(G + C_{\varepsilon 3}G_\mathrm{B}) - C_{\varepsilon 2}\varepsilon)\,\frac{\varepsilon}{k} \tag{7}$$

the generation of turbulence due to the shear stresses and the buoyancy force is calculated as follows:

$$G = \frac{\mu_\mathrm{t}}{\rho}\frac{\partial u_j}{\partial x_i}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\left(k + \frac{\mu_\mathrm{t}}{\rho}\frac{\partial u_k}{\partial x_k}\right), \quad G_\mathrm{B} = -\frac{\mu_\mathrm{t}}{\rho}\frac{1}{\mathrm{Pr}_\mathrm{t}}\frac{g_j}{\rho}\frac{\partial \rho}{\partial x_j}\,.$$

The eddy viscosity is found from the Kolmogorov–Prandtl formula:

$$\mu_\mathrm{t} = C_\mu\,\rho\,\frac{k^2}{\varepsilon}\,.$$

In the calculations, we used the constants $C_\mu = 0.09$, $C_{\varepsilon 1} = 1.30$, $C_{\varepsilon 2} = 1.92$, $C_{\varepsilon 3} = 1.0$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $\mathrm{Pr}_\mathrm{t} = 0.7$, and $\mathrm{Sc}_\mathrm{t} = 0.7$.

It is known [14, 15] that the standard k–ε model of turbulence does not give a qualitative description of flow in the region adjacent to the fuel surface where the flow is not fully turbulent. Moreover, this model does not allow adequate representation of the width of a round jet [16, 17] or an ascending torch [18–20]. This manifests itself as the overestimation of the temperature and velocity on the flow axis and the underestimation of its cross-section area. Correspondingly, the height and width of the flame are also distorted. To overcome this drawback, a number of modifications of this class of turbulence models are used. For example, corrections to Eq. (7) for the dissipation rate [16, 17], other sets of constants [18], and also variants of an algebraic model of Reynolds stresses [19, 20] have been suggested. In the present work, with this in mind, we used $C_{\varepsilon 1} = 1.30$ instead of the standard value $C_{\varepsilon 1} = 1.44$, which made it possible to substantially improve agreement between the calculated and measured quantities.

In modeling of combustion, we took a two-stage successive scheme of fuel oxidation, which involves three reactions. In the first stage, fuel decomposes to form water vapor, carbon monoxide, and free carbon in the form of soot:

$$\mathrm{C}_{n_\mathrm{C}}\mathrm{H}_{n_\mathrm{H}}\mathrm{O}_{n_\mathrm{O}} + \left(\frac{n_\mathrm{C}}{2}(1 - \chi_\mathrm{C}) + \frac{n_\mathrm{H}}{4} - \frac{n_\mathrm{O}}{2}\right)\mathrm{O}_2 \rightarrow (1 - \chi_\mathrm{C})\,n_\mathrm{C}\mathrm{CO} + \chi_\mathrm{C} n_\mathrm{C}\mathrm{C} + \frac{n_\mathrm{H}}{2}\,\mathrm{H_2O}\,. \tag{8}$$

In the second stage, carbon monoxide and soot are oxidized to carbon dioxide:

$$\mathrm{CO} + \frac{1}{2}\,\mathrm{O}_2 \rightarrow \mathrm{CO}_2\,, \tag{9}$$

$$\mathrm{C} + \mathrm{O}_2 \rightarrow \mathrm{CO}_2\,. \tag{10}$$

The rates of the reactions were determined using the model of vortex disintegration [21]

$$\dot r^{(1)} = C_\mathrm{R}^{(1)}\,\frac{\varepsilon}{k}\min\left(Y_\mathrm{fuel}, \frac{Y_{\mathrm{O}_2}}{s_{\mathrm{O}_2}^{(1)}}\,\frac{Y_\mathrm{fuel}s_{\mathrm{O}_2}^{(1)}}{Y_\mathrm{fuel}s_{\mathrm{O}_2}^{(1)} + Y_\mathrm{CO}s_{\mathrm{O}_2}^{(2)} + Y_\mathrm{C}s_{\mathrm{O}_2}^{(3)}}\right),$$

$$\dot r^{(2)} = C_\mathrm{R}^{(2)}\,\frac{\varepsilon}{k}\min\left(Y_\mathrm{CO}, \frac{Y_{\mathrm{O}_2}}{s_{\mathrm{O}_2}^{(2)}}\,\frac{Y_\mathrm{CO}s_{\mathrm{O}_2}^{(2)}}{Y_\mathrm{fuel}s_{\mathrm{O}_2}^{(1)} + Y_\mathrm{CO}s_{\mathrm{O}_2}^{(2)} + Y_\mathrm{C}s_{\mathrm{O}_2}^{(3)}}\right),$$

$$\dot{r}^{(3)} = C_{\mathrm{R}}^{(3)} \frac{\varepsilon}{k} \min \left(Y_{\mathrm{C}}, \frac{Y_{\mathrm{O}_2}}{s_{\mathrm{O}_2}^{(3)}} \frac{Y_{\mathrm{C}} s_{\mathrm{O}_2}^{(3)}}{Y_{\mathrm{fuel}} s_{\mathrm{O}_2}^{(1)} + Y_{\mathrm{CO}} s_{\mathrm{O}_2}^{(2)} + Y_{\mathrm{C}} s_{\mathrm{O}_2}^{(3)}} \right),$$

where the superscripts (1), (2), and (3) correspond to reactions (8), (9), and (10). Oxidation of soot at a temperature below 600 K was taken to be insignificant. In calculations of a propane flame in air, the best agreement with the measured concentration profiles of the main components was obtained at $C_{\mathrm{R}}^{(1)} = 4.0$, $C_{\mathrm{R}}^{(2)} = 1.0$, and $C_{\mathrm{R}}^{(3)} = 2.0$. The right-hand sides in (2) of component transfer, which correspond to reactions (8)–(10), have the form

$$\dot{R}_{\mathrm{fuel}} = -\dot{r}^{(1)} , \quad \dot{R}_{\mathrm{CO}} = s_{\mathrm{CO}}^{(1)} \dot{r}^{(1)} - \dot{r}^{(2)} , \quad \dot{R}_{\mathrm{C}} = s_{\mathrm{C}}^{(1)} \dot{r}^{(1)} - \dot{r}^{(3)} , \quad \dot{R}_{\mathrm{O}_2} = -s_{\mathrm{O}_2}^{(1)} \dot{r}^{(1)} - s_{\mathrm{O}_2}^{(2)} \dot{r}^{(2)} - s_{\mathrm{O}_2}^{(3)} \dot{r}^{(3)} ,$$

$$\dot{R}_{\mathrm{CO}_2} = s_{\mathrm{CO}_2}^{(2)} \dot{r}^{(2)} + s_{\mathrm{CO}_2}^{(3)} \dot{r}^{(3)} , \quad \dot{R}_{\mathrm{H}_2\mathrm{O}} = s_{\mathrm{H}_2\mathrm{O}}^{(1)} \dot{r}^{(1)} .$$

The rate of formation of soot was determined using the empirical relation [22]

$$\rho \dot{r}_{\mathrm{S.F}} = C_{\mathrm{S.F}} P_{\mathrm{fuel}} \phi^n \exp \left(-\frac{E_{\mathrm{S.F}}}{RT} \right),$$

which relates the quantity $\dot{r}_{\mathrm{S.F}}$ to the mixture temperature T and the concentrations of the fuel and oxygen (in terms of the partial pressure of the fuel P_{fuel} and the quantity $\varphi = \left(Y_{\mathrm{fuel}} s_{\mathrm{O}_2}^{(1)} / Y_{\mathrm{O}_2} \right)$. The coefficient χ_{C} is calculated as

$$\chi_{\mathrm{C}} = \min \left(1, \frac{\dot{r}_{\mathrm{S.F}}}{n_{\mathrm{C}} M_{\mathrm{C}}} \frac{M_{\mathrm{fuel}}}{\dot{r}^{(1)}} \right).$$

The numerical values $C_{\mathrm{S.F}} = 2.0$ sec/m^2, $n = 3$ [22], and $E_{\mathrm{S.F}}/R = 10^4$ K used in this work allowed obtaining 0.02 to 0.06 g of soot per gram of burned propane in the flow of products, which is in agreement with the data of measurements [23].

Thermal-Radiation Transfer. The problem of modeling thermal-radiation transfer is reduced to determination of the divergence $\partial q_j^{\mathrm{r}} / \partial x_j$ of the radiation flow (the right-hand side of energy equation (4)) at each point of the volume and the radiation heat flux incident on enclosing surfaces. In this work, thermal-radiation transfer is considered in the approximation of a gray medium. The calculations showed that if the spectrum-averaged effective coefficient of absorption K_{abs} is calculated properly, the suggested model represents both the temperature field in the flame zone and the emitted radiation flows rather adequately. We note that the scattering of infrared radiation on submicron soot particles which are formed in hydrocarbon flames is insignificant [1]. It is assumed that solid surfaces emit self-radiation and reflect incident radiation diffusely.

Thermal-radiation transfer in the assigned direction in a grey nonscattering medium is described by the following equation [2–4]:

$$\frac{dI}{ds} = -K_{\mathrm{abs}} (I - I_{\mathrm{b}}) , \quad I_{\mathrm{b}} = 4\sigma T^4 . \tag{11}$$

The divergence of the radiation flux necessary for solution of the energy equation (4) has the form

$$\frac{\partial q_j^{\mathrm{r}}}{\partial x_j} = -4K_{\mathrm{abs}} (E_{\mathrm{b}} - E) ,$$

where $E = \frac{1}{4} \int_0^{4\pi} I d\omega$ and $E_{\mathrm{b}} = \frac{1}{4} \int_0^{4\pi} I_{\mathrm{b}} d\omega$ are found by integration of the intensity with respect to the whole solid angle ω.

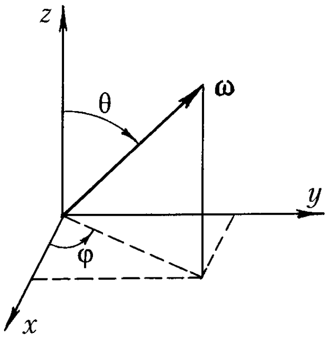

Fig. 1. Angular coordinates of the direction of photon flight.

Statistical method. The main method of calculation used in the present work is the statistical method (Monte Carlo method), which has been applied to radiation emitted by both the internal control volumes and the boundary surface elements of a computational grid. In both cases, the method consists of two stages. In consideration of the internal emission of radiation, we assume that:

1. Each internal control volume of the computational grid emits a rather large number of "photons" (portions of energy) the total energy of which is $4K_{\text{abs}}\sigma T^4 \Delta V \Delta t$. The directions of escape of photons are random. The probability of selection of each direction is uniformly distributed over the whole solid angle. In emission of a photon, the substance in the mesh loses a portion of energy which is equal to the energy of the photon.

2. The history of each photon emitted and moving along rectilinear trajectories is tracked. The photon can be absorbed, and then observation over the photon is stopped and its energy is added to the energy of the substance in the mesh. The photon can follow the neighboring mesh, where its history is tracked similarly. Finally, it can reach the region boundary (a solid wall or free escape to an unbounded space). In the latter case, one chooses between the absorption and the reflection of the photon. The probability of absorption is in proportion to the emissivity of the boundary surface ε_{w}. In the case of absorption, the photon energy makes a contribution to the heat flux absorbed by the surface.

In modeling the emission of radiation by bounding surfaces, we assume that:

1. Each boundary surface element of the computational grid emits a certain rather large number of photons, the total energy of which is $\varepsilon_{\text{w}}\sigma T^4 \Delta S \Delta t$. The directions of escape of photons are random. Since a diffusely radiating surface is taken, the probability selection of each direction is uniformly distributed over half of the solid angle which faces the interior of the region. In emission of the photon, its energy is subtracted from the radiation energy absorbed by the surface at this time step.

2. The history of each photon emitted and moving along rectilinear trajectories is tracked in a similar way.

The divergence of the radiation flux is calculated as the difference of the emitted and absorbed energies divided by $\Delta V \Delta t$.

We present the main features of implementation of the method in this work. Let r_0, r_φ, r_θ, and r_{abs} be random quantities uniformly distributed from 0 to 1. The coordinates of the point of photon escape were taken to be equiprobable inside each mesh of the grid:

$$x^0 = x_{i-1} + r_0\,(x_i - x_{i-1})\,,\ y^0 = y_{j-1} + r_0\,(y_j - y_{j-1})\,,\ z^0 = z_{k-1} + r_0\,(z_k - z_{k-1})\,,$$

where x_i, y_j, and z_k are the coordinates of the boundaries of grid meshes. The direction cosines of the vector $\boldsymbol{\omega} = \omega_x\mathbf{i} + \omega_y\mathbf{j} + \omega_z\mathbf{k}$ are expressed in terms of the angles θ and φ shown in Fig. 1:

$$\omega_x = \sin\theta\cos\varphi\,,\ \omega_y = \sin\theta\sin\varphi\,,\ \omega_z = \cos\theta\,.$$

The angles θ and φ are found from the conditions

$$\cos\theta = 2r_\theta - 1\,,\quad \varphi = 2\pi r_\varphi\,.$$

The direction of flight and the coordinates of entry of the photon to grid meshes are determined from the equation of the line

$$\frac{x - x^0}{\omega_x} = \frac{y - y^0}{\omega_y} = \frac{z - z^0}{\omega_z} ,$$

where x^0, y^0, and z^0 are the coordinates of the point of photon emission or the point of appearance of a photon flying from outside in a given control volume. The path length of the photon till its absorption is

$$L_{\text{abs}} = \frac{1}{K_{\text{abs}}\,(x_{i-1/2}, y_{j-1/2}, z_{k-1/2})} \ln \frac{1}{1 - r_{\text{abs}}} .$$

If L_{abs} turns out to be smaller than the length to the neighboring grid mesh along the direction of flight, the photon is absorbed.

The number of emitted photons was taken to be in proportion to the difference between the energy emitted at the point with a temperature T and the energy emitted at the lowest (background) temperature T_0:

$$N_{\text{vol}\,i,j,k} = N_{\text{vol max}} \frac{K_{\text{abs}}\,(T^4 - T_0^4)\,\Delta V}{\sum\limits_{\text{vol}\,i,j,k} K_{\text{abs}}\,(T^4 - T_0^4)\,\Delta V}$$

for the internal control volumes and

$$N_{\text{surf}\,i,j,k} = N_{\text{surfmax}} \frac{\varepsilon_{\text{w}}\,(T^4 - T_0^4)\,\Delta S}{\sum\limits_{\text{surf}\,i,j,k} \varepsilon_{\text{w}}\,(T^4 - T_0^4)\,\Delta S}$$

for the boundary surface elements. Thus, photons are not emitted by a cold medium, which allows one to avoid a non-physical drop in the temperature below the lowest (background) value. The total number of photons $N_{\text{vol max}} + N_{\text{surf max}}$ was varied within $5{\cdot}10^4$–$2{\cdot}10^6$ depending on the specific problem. The energy of each photon was $4K_{\text{abs}}\sigma T^4 \Delta V \Delta t$ divided by the number of photons.

Flow method. We note that the flow method is the simplest and thus most widespread method in engineering practice [2]. In this work, the method was used to compare the results of calculation by it and by the Monte Carlo method. We recall that the flow method is deduced on the assumption that the intensity of radiation inside each of the six segments of the solid angle is constant (the axes of each segment are parallel to the coordinate axes x, y, z) [2]. In this method, the density of radiation energy $E = (E_x + E_y + E_z)/3$ is determined by solution of the one-dimensional equations

$$\frac{\partial}{\partial x_j} \frac{1}{mK_{\text{abs}}} \frac{\partial E_i}{\partial x_j} + mK_{\text{abs}}\,(E_{\text{b}} - E_i) = 0 , \quad i = x, y, z , \quad m \approx 1.2 , \tag{12}$$

for each of the components E_x, E_y, and E_z with boundary conditions of the form

$$\pm \frac{4}{3m^2 K_{\text{abs}}} \frac{\partial E_i}{\partial x_j} = \frac{2\varepsilon_{\text{w}}}{2 - \varepsilon_{\text{w}}} \left[\frac{2}{3m} \left(E_i + \left(\frac{3}{4m} - \frac{1}{2} \right) (E_j + E_k) \right) - E_{\text{b,w}} \right] , \tag{13}$$

where the plus sign is taken on the left boundary and the minus sign is taken on the right boundary and $E_{\text{b,w}}$ is calculated at the wall temperature. The resultant heat flux to the wall is determined from the left-hand side of (13).

Radiation Properties of the Medium. The effective coefficient of absorption is determined by the contribution of the gaseous (H_2O, CO_2, CO) and condensed (soot) combustion products and the unburned fuel.

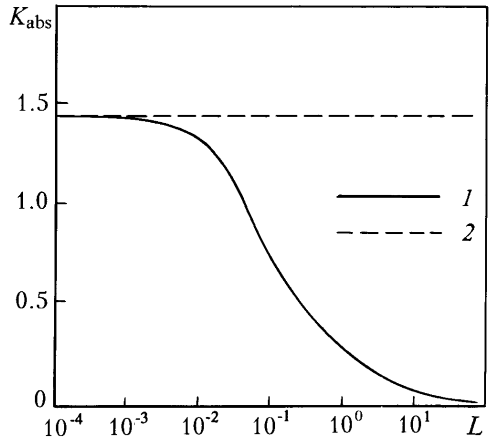

Fig. 2. Dependence of the effective coefficient of absorption on the path length of radiation: 1) calculation from (15); 2) calculation from (16). K_{abs}, 1/m; L, m.

Mixture of CO_2 *and* H_2O. When the gray-medium approximation is used, the effective value of the absorption coefficient in each mesh of the computational grid must be determined so that the value of the radiating capacity is close to that obtained from a spectral analysis. In this work, to calculate the radiating capacity of the gas volume we used the model of the weighted sum of gray gases (see [1, 4, 24] and others)

$$\varepsilon_{CO_2+H_2O} = \sum_{i_g=0}^{3} a_{g,i_g}(T)\,(1-\exp(k_{g,i_g}(P_{CO_2}+P_{H_2O})\,L))\,, \tag{14}$$

where the gas phase is represented by a set of three gray "gases" (i_g = 1, 2, 3) and one transparent (i_g = 0) "gas" with effective properties. The weight factors a_{g,i_g} depend on temperature and are approximated by the fourth-degree polynomials

$$a_{g,i_g}(T) = \sum_{j=0}^{3} b_{g,i_g,j}\,T^j\,, \quad i_g = 0, 1, 2, 3\,.$$

The numerical values of the polynomial coefficients $b_{g,i_g,j}$ and the absorption coefficients k_{g,i_g} are given in [25].

For a mesh of the computational grid with dimensions Δx, Δy, and Δz, a volume $\Delta V = \Delta x\Delta y\Delta z$, and an area of the side surface $\Delta S = 2(\Delta x\Delta y + \Delta x\Delta z + \Delta y\Delta z)$, we took

$$L = 3.6\cdot\frac{\Delta V}{\Delta S} = \frac{1.8}{1/\Delta x + 1/\Delta y + 1/\Delta z}\,.$$

The effective value of the absorption coefficient is determined as

$$K_{abs,CO_2+H_2O} = \frac{1}{L}\ln\left(\frac{1}{1-\varepsilon_{CO_2+H_2O}}\right). \tag{15}$$

In the optically transparent approximation, i.e., at low values of $\left(P_{CO_2}+P_{H_2O}\right)L$, we have

$$K_{abs,CO_2+H_2O} = \sum_{i_g=0}^{3} a_{g,i_g}(T)\,k_{g,i_g}\,. \tag{16}$$

Figure 2 gives the dependence of the effective coefficient of absorption on the path length of radiation at parameters typical of the flame zone (T = 1300 K, $Y_{CO_2} = Y_{H_2O}$ = 0.1). It is seen that calculation in the optically trans-

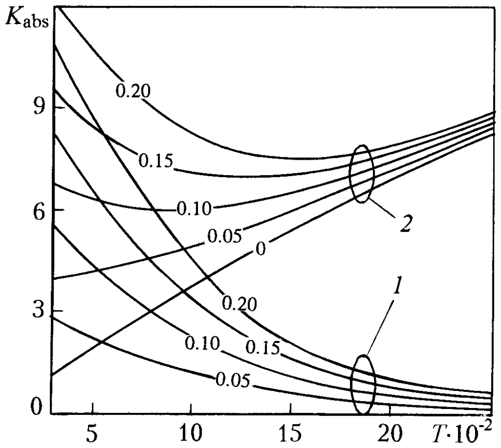

Fig. 3. Effective coefficient of absorption of the mixture of CO_2, H_2O, and soot: f_V = 0 (1) and $2\cdot10^{-6}$ (2). Numbers in the figure — mass fractions of CO_2 and H_2O (they are assumed to be equal). K_{abs}, 1/m; T, K.

parent approximation (16) is justified only for grids with a characteristic dimension of meshes less than 1 cm. In calculations on larger grids, one must use relation (15). We note that the effective coefficient of absorption decreases substantially with increase in the radiation path length. As is shown in [26], the effective coefficient of absorption calculated from formulas (14) and (15) on the basis of the data from [25] is in good agreement with the result of a more accurate spectral calculation by the wide-band model.

Soot. The absorption coefficient for soot was calculated using the relation

$$K_{abs,s} = f_V \sum_{i_s=1}^{2} a_{s,i_s}(T)\, k_{s,i_s} , \tag{17}$$

where soot is represented by a combination of two gray "gases" (i_s = 1, 2). The weight factors a_{s,i_s} depend on temperature and are approximated by the fourth-degree polynomials

$$a_{s,i_s}(T) = \sum_{j=0}^{3} b_{s,i_s,j}\, T^j , \quad i_s = 1, 2 .$$

The numerical values of the polynomial coefficients $b_{s,i_s,j}$ and the absorption coefficients k_{s,i_s} are given in [27, 28].

We note that the absorption coefficient for soot can be obtained from the Mie theory in the Rayleigh limit of small spherical particles. To calculate the spectrum-mean coefficient, in [29] it was suggested to use the following expression:

$$K_{abs,s} = 3.72\cdot\frac{C_0}{C_2} f_V T , \tag{18}$$

where $C_2 = 1.44\cdot10^{-2}$ m·K and C_0 is the empirical constant from the range 2–6 [29] or an even wider one [1], which depends on the complex refraction index of soot. The following values are given in [1]: C_0 = 3.7–7.5 for carbon flames, C_0 = 6.3 for oil, C_0 = 4.9 for propane, and C_0 = 4.0 for acetylene. One can assure oneself that the data of [27] approximately correspond to C_0 = 5.0 and the data of [28] correspond to C_0 = 7.0. By and large, we should point out an appreciable disagreement of the absorption coefficients suggested by different authors.

CO and unburned fuel. The absorption coefficients $K_{abs,CO}(T, P_{CO})$ and $K_{abs,CH_4}(T, P_{CH_4})$ for CO and methane were calculated in the optically transparent approximation from the data of [30].

In view of the shortage of experimental information on the coefficients of absorption of hydrocarbons, it was assumed that the coefficient of absorption $K_{abs,fuel}(T, P_{fuel})$ of hydrocarbon fuels different from methane equals the coefficient of absorption of methane $K_{\mathrm{abs,CH_4}}(T,\ P_{\mathrm{CH_4}})$. Because of the low partial pressure of the fuel vapor, the error introduced by this assumption is small.

The effective coefficient of absorption of a mixture. The quantity K_{abs} was calculated as follows:

$$K_{\mathrm{abs}} = K_{\mathrm{abs,CO_2+H_2O}}\,(T, P_{\mathrm{CO_2}}, P_{\mathrm{H_2O}}, L) + K_{\mathrm{abs,s}}\,(T, f_V) + K_{\mathrm{abs,CO}}\,(T, P_{\mathrm{CO}}) + K_{\mathrm{abs,fuel}}\,(T, P_{\mathrm{fuel}})\ . \tag{19}$$

The dependence of the absorption coefficient on temperature for mixtures of different compositions is shown in Fig. 3. The coefficients of absorption of the gas components decrease as the temperature increases, whereas the coefficient of absorption of soot increases linearly. In this case, the resultant dependence for a mixture can have a minimum. In the region of relatively low temperatures (below 1000 K), the contribution of the gas components to the absorption coefficient is comparable to or exceeds the contribution of the soot. At higher temperatures typical of the flame zone and at the volume fraction of the aerosol $f_V = 2{\cdot}10^{-6}$, indicated in Fig. 2, the contribution of the soot is substantially higher.

Account for turbulent fluctuations. In a fluctuating turbulent flow, an averaged equation of radiation transfer (11) takes on the form

$$\frac{d\overline{I}}{ds} = \overline{K_{\mathrm{abs}} I_{\mathrm{b}}} - \overline{K_{\mathrm{abs}} I}\ . \tag{20}$$

Just as in [31], we assume that the effect of local fluctuations of the absorption coefficient K_{abs} on the transmitted and absorbed radiation is insignificant, i.e., $\overline{K_{\mathrm{abs}} I} \approx \overline{K}_{\mathrm{abs}} \overline{I}$. On the contrary, in the term for the averaged emission of radiation of the mixture of gases and soot $\overline{K_{\mathrm{abs}} I_{\mathrm{b}}}$ which is proportional into $\overline{K_{\mathrm{abs}} T^4}$, the instantaneous values are in correlation. As a rule, in calculations it is assumed that $\overline{K_{\mathrm{abs}} T^4} = \overline{K_{\mathrm{abs}}}\ \overline{T}^4$, which means neglect of the turbulent fluctuations of the temperature and the absorption coefficient. This can lead to an appreciable error if the amplitude of the fluctuations is rather large. For example, the measurements of [32, 33] showed that the mean amplitude of turbulent fluctuations in a propane flame in air above a burner of diameter of 0.3 m can reach 50% of the mean temperature. In this case one must take into account the effect of fluctuations on the emission of radiation. We note that the absorption coefficient depends on the temperature of the medium and its composition (concentration of gas components and volume fraction of soot). Just as in [34], in the present work, the effect of fluctuations on the quantity $\overline{K_{\mathrm{abs}} T^4}$ is considered without regard for the fluctuations of mixture composition.

Resolution of $T = \overline{T} + T'$ and $K_{\mathrm{abs}} = \overline{K}_{\mathrm{abs}} + K'_{\mathrm{abs}}$ into the mean and fluctuation components with subsequent substitution into $\overline{K_{\mathrm{abs}} T^4}$ and averaging yields

$$\overline{K_{\mathrm{abs}} T^4} = \overline{K_{\mathrm{abs}}}\ \overline{T}^4 \left(1 + 6\,\frac{\overline{T'^2}}{\overline{T}^2} + 4\,\frac{\overline{T'^3}}{\overline{T}^3} + \frac{\overline{T'^4}}{\overline{T}^4} + 4\,\frac{\overline{K'_{\mathrm{abs}} T'}}{\overline{K_{\mathrm{abs}}}\ \overline{T}} + 6\,\frac{\overline{K'_{\mathrm{abs}} T'^2}}{\overline{K_{\mathrm{abs}}}\ \overline{T}^2} + 4\,\frac{\overline{K'_{\mathrm{abs}} T'^3}}{\overline{K_{\mathrm{abs}}}\ \overline{T}^3} + \frac{\overline{K'_{\mathrm{abs}} T'^4}}{\overline{K_{\mathrm{abs}}}\ \overline{T}^4} \right), \tag{21}$$

where the bracketed expression reflects the effect of turbulent fluctuations, with terms (from fifth to eighth) accounting for the correlation of the fluctuations of the absorption coefficient and the temperature. In what follows, we will take into account only the contribution of correlations of lowest order, i.e., $\overline{T'^2}$ and $\overline{T' K'_{\mathrm{abs}}}$, which should be approximately expressed in terms of the averaged characteristics of flow.

To calculate $\overline{T' K'_{\mathrm{abs}}}$ we represent the dependence $K_{\mathrm{abs}}(T) = K_{\mathrm{abs}}(\overline{T} + T')$ in the form of the series

$$K_{\mathrm{abs}} = K_{\mathrm{abs}}\,(\overline{T}) + T'\left.\frac{\partial K_{\mathrm{abs}}}{\partial T}\right|_{\overline{T}} + \left.\frac{T'^2}{2}\,\frac{\partial^2 K_{\mathrm{abs}}}{\partial T^2}\right|_{\overline{T}} + \dots\ .$$

Using this relation, we can calculate the mean value of $\overline{K_{\mathrm{abs}}}$ and the fluctuation component $K'_{\mathrm{abs}} = K_{\mathrm{abs}} - \overline{K_{\mathrm{abs}}}$ of the absorption coefficient. Multiplication by T' and subsequent averaging yield

$$\overline{T'K'_{\text{abs}}} = \overline{T'^2}\,\frac{\partial K_{\text{abs}}}{\partial T}\bigg|_{\bar T} + \frac{\overline{T'^3}}{2}\,\frac{\partial^2 K_{\text{abs}}}{\partial T^2}\bigg|_{\bar T} + \ldots \approx \overline{T'^2}\,\frac{\partial K_{\text{abs}}}{\partial T}\bigg|_{\bar T}\,.$$

Neglecting the correlations of high order in (21), we have

$$\overline{K_{\text{abs}}T^4} = \overline{K_{\text{abs}}}\,\bar T^4\left(1 + C\,6\,\frac{\overline{T'^2}}{\bar T^2}\left(1 + \frac{2}{3}\,\frac{\bar T}{\overline{K_{\text{abs}}}}\,\frac{\partial K_{\text{abs}}}{\partial T}\bigg|_{\bar T}\right)\right), \tag{22}$$

where C is a constant which in the present work was taken to be equal to 4. We note that the derivative $\partial K_{\text{abs}}/\partial T$ can change its sign depending on the composition and temperature of the mixture. If the volume fraction of soot is small and the absorption coefficient is determined by the contribution of CO_2 and H_2O, then $\partial K_{\text{abs}}/\partial T < 0$ (see Fig. 2, $f_V = 0$). In the case of a large volume fraction of soot and at a rather high temperature, we have $\partial K_{\text{abs}}/\partial T > 0$ (see Fig. 2, $f_V = 2\cdot 10^{-6}$, $T > 1500$ K). The calculations made within the range of parameters typical of a flame showed that the role of the term involving $\partial K_{\text{abs}}/\partial T$ is insignificant.

To calculate $\overline{T'^2}$ we used the equation of transfer of the root-mean-square fluctuation [13]

$$\frac{\partial \rho \overline{T'^2}}{\partial t} + \frac{\partial \rho u_j \overline{T'^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_{\text{t}}}{\text{Pr}_{\text{t}}}\right)\frac{\partial \overline{T'^2}}{\partial x_j} + 2\,\frac{\mu_{\text{t}}}{\text{Pr}_{\text{t}}}\,\frac{\partial \bar T}{\partial x_j}\,\frac{\partial \bar T}{\partial x_j} - C_{\text{t}}\,\rho \overline{T'^2}\,\frac{\varepsilon}{k}\,, \tag{23}$$

where $C_{\text{t}} = 2.0$. Equation (23) is solved simultaneously with other equations of transfer ((1)–(6)). We note that for the considered type of flame the flow directly above the burner nozzle or above the fuel surface is not fully turbulent, since the velocity of both the fuel and the entrained air is small. By virtue of this fact, the assumptions made in derivation of relation (22) can fail. Therefore, the correction to the quantity $\overline{K_{\text{abs}}}\,\bar T^4$ introduced into (22) was allowed for only when the local turbulent Reynolds number $k^2/\varepsilon\nu$ exceeded 10^2.

CONCLUSIONS

We have analyzed the methods of calculation of thermal-radiation transfer which are used in modeling of turbulent diffusion flames. The advantages of the statistical approach to modeling of radiation transfer have been revealed; within the framework of this approach, on the one hand, splitting of the solid angle is not used and no distinguished directions of radiation transfer arise and, on the other hand, no assumptions on the isotropic nature of radiation are made.

The suggested implementation of the statistical method in combination with the equations of turbulent flow and combustion of a multicomponent mixture formed in combustion of hydrocarbons in air has been presented. A description of the method for calculation of the effective spectrum-averaged coefficient of absorption has been given for a mixture of absorbing gases and soot. The effect of turbulent temperature fluctuations on the emission of thermal radiation has been taken into account.

The formulated algorithm was used in modeling natural-convection turbulent diffusion flames above a gas burner and above the surface of a liquid fuel.

NOTATION

C_P, heat capacity at constant pressure, J/(kg·K); C_μ, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, $C_{\varepsilon 3}$, σ_k, σ_ε, and C_{t}, constants of the turbulence model; $C_{\text{R}}^{(i)}$, rate constant of the ith reaction; E, radiation-energy density, W/m^2; $E_{\text{S.F}}$, $C_{\text{S.F}}$, and n, parameters of the soot-formation model, J/mole and sec/m^2; f_V, volume fraction of soot; g, free-fall acceleration, m/sec^2; G and G_{B}, generation of turbulence due to the shear stresses and the buoyancy force respectively, m^2/sec^3; h, enthalpy of the mass unit, J/kg; I, radiation intensity, W/(m^2·sr); s, distance along a certain direction of radiation transfer, m; k, kinetic energy of turbulence, m^2/sec^2; K_{abs}, coefficient of thermal-radiation absorption, 1/m; $k_{\text{g},i_{\text{g}}}$, $a_{\text{g},i_{\text{g}}}$, $b_{\text{g},i_{\text{g}},j}$, $k_{\text{s},i_{\text{s}}}$, $a_{\text{s},i_{\text{s}}}$, and $b_{s,i_s,j}$, parameters for calculation of the radiating capacity of the mixture of CO_2, H_2O, and soot; L, mean path length of radiation, m; L_{abs}, path length of a photon till absorption, m; M_α, molar mass of the α-component, kg/mole; n_C, n_H, and n_O, number of carbon, hydrogen, and oxygen atoms, respectively, in a fuel molecule; N_{vol} and N_{surf}, number of photons in the statistical method; Pr, Prandtl number; p, dynamic pressure, Pa; P, total pressure, Pa; P_α, partial pressure of the α-component, Pa; g^r, radiation heat flux, W/m^2; $\dot{r}^{(i)}$, rate of the ith reaction, 1/sec; $\dot{r}_{S.F}$, rate of formation of soot, 1/sec; R, universal gas constant, J/(mole·K); R_α, rate of formation of the α-component due to combustion, 1/sec; $s_\alpha^{(i)}$, mass stoichiometric coefficients for the α-component in the ith reaction; Sc, Schmidt number; t, time, sec; T, temperature, K; x_j and u_j, coordinates and projections of velocity, m and m/sec; x, y, z, spatial coordinates, m; Y_α, mass fraction of the α-component, kg/kg; δ_{ij}, Kronecker symbol; $\Delta h^0_{f\alpha}$, standard enthalpy of formation of the α-component, J/kg; Δt, time step, sec; ΔV and ΔS, volume and area of the side surface of the grid mesh, m^3 and m^2; Δx, Δy, and Δz, dimensions of the grid mesh, m; ε, dissipation rate of turbulent energy, m^2/sec^3; $\varepsilon_{H_2O+CO_2}$, radiating capacity of the mixture of H_2O and CO_2; ε_w, emissivity of the boundary surface; $\boldsymbol{\omega}$, unit vector in the direction of photon flight; **i**, **j**, **k**, unit vectors of the coordinate system; ϕ, excess-fuel coefficient; φ and θ, polar and azimuth angles, rad; χ_C, carbon fraction in a fuel molecule expended on forming soot; μ, dynamic viscosity, Pa·sec; ρ, density, kg/m^3; σ, Stefan–Boltzmann constant, W/(m^2·K^4); τ_{ij}, components of the stress tensor, Pa; ω, solid angle, sr. Sub- and superscripts: abs, absorption; b, black body; B, buoyancy; fuel, fuel; g, gas; (i), reaction number; i, j, and k, number of the grid mesh; R, reaction; r, radiation; S.F, soot formation; s, soot; surf, boundary surface element; t, turbulent; vol, internal control volume; w, solid wall; α, mixture component; 0, surrounding air; overbar, time-averaging of fluctuating quantities; prime, fluctuations; f, flame zone; max, maximum.

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