

teristics of the furnace medium of powdered coal furnaces in any zone of the furnace chamber.

NOTATION

w , c , and t , velocity, specific heat, and temperature of the combustion products, respectively; E_{res} , resultant heat flux over the surface of the volume considered; q , heat released per unit volume; Q_7^w , lowest heat of combustion of the working mass of fuel; n and m , fraction of the fuel and recirculation per layer, respectively; β , degree of burning of the fuel in the zone; $\Delta\beta$, degree of burning in a specified zone from the combustion of the fuel introduced into previous zones; t_1 , t_2 , c_1 , and c_2 , temperature and heat capacity of the combustion products at the entrance and the exit from the zone, respectively; t_g , c_g , and r , temperature, heat capacity, and fraction of the recirculation gases; B_p , theoretical fuel flow rate; ψ , thermal efficiency; F , surface bounding the zone; Vc_2 , total heat capacity of the combustion products for t_2 ; $\Delta\epsilon_t = \epsilon_{tcal} - \epsilon_{texp}$, difference between the theoretical degree of brightness of the surface volume and the experimental value; r_t , r_{CO_2} , and r_{H_2O} , total volume fraction of triatomic gases and the volume fraction of CO_2 and H_2O , respectively; μ_a , dimensionless concentration of ash particles; d_a , effective diameter of the ash particles; κ_1 and κ_2 , quantities which take into account the concentration of coke particles in the combustion product; p_D , total partial pressure of the gases; T , temperature of the combustion products; $\mu_c\mu_{ca}$, dimensionless and actual concentration of coke particles; and σ_0 , emissivity of blackbody.

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PROBABILISTIC MODELING OF VIBRATIONALLY NONEQUILIBRIUM DIATOMIC GASES IN THE THEORY OF RADIATION TRANSFER

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The radiation transfer in a vibrationally nonequilibrium diatomic gas is described by a system of equations which can be reduced to one integrodifferential equation for the vibrational energy density. A method for the numerical solution of this equation by using the theory of Markov chains is proposed in the paper.

The investigation of radiation transfer in nonequilibrium gases is closely associated with such areas of application as spectroscopy, low-temperature plasmas, molecular gasdynamic lasers, radiation gasdynamics, and physics of the upper layers of a planetary atmosphere. In the general case, the problem reduces to solving a system of equations of Boltzmann type for material particles and photons [1, 2]. Obtaining concrete results by direct integration of the system of equations is hence a very complex mathematical problem. Hence, examination of such physical situations when the problem allows of specific simplifications is of interest. The present paper is devoted to an investigation of radiation energy transfer in nonequilibrium diatomic heteronuclear gases (CO , HCl , NO , etc., for example) both because of the relative simplicity of configuration of diatomic molecules and the practical importance of such gases for radiation gasdynamics and atmospheric optics problems. Radiation processes exert a substantial effect, together with inelastic collisions on the population of the vibrational-rotational molecule levels at reduced pressures of the radiating medium $p \sim 10^{-4}$ - 10^{-3}

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and the temperatures $T \sim 1-3 \cdot 10^3 \text{K}$ when the maximum of the Planck functions is in the frequency range corresponding to vibrational-rotational transitions. The emergence of radiation outside the boundaries of the emitting volume in this case results in spoilage of the local thermodynamic equilibrium. However, a representation about the local equilibrium within separate degrees of freedom [3, 4], and particularly, about the vibrational temperature $T_v(\mathbf{r})$ which differs from the translational $T(\mathbf{r})$ (the temperature of the rotational degrees of freedom also equals $T(\mathbf{r})$), can be introduced for a broad class of problems. The radiation characteristics of such a partially equilibrium medium are determined by the radiation transfer equation in which the source function depends on $T_v(\mathbf{r})$ or the equivalent parameter $\varepsilon(\mathbf{r})$, the gas vibrational energy density. In turn, a kinetic equation must be written for $\varepsilon(\mathbf{r})$, where besides the relaxation term, a term describing the influence of the radiation transitions should be present.

Considering the diatomic molecules in the "quantum oscillator-rigid rotator" approximation, the following system of equations can be written for the gas vibrational energy density $\varepsilon(\mathbf{r})$ and the spectral intensity $I(\mathbf{k}, \mathbf{r})$:

$$n \nabla I(\mathbf{k}, \mathbf{r}) = k_v(\mathbf{r}) (I_v^0(\mathbf{r}) - I(\mathbf{k}, \mathbf{r})), \quad (1)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}(\mathbf{r}) \nabla \right) \varepsilon(\mathbf{r}) = \frac{\varepsilon^0(\mathbf{r}) - \varepsilon(\mathbf{r})}{\tau^0(\mathbf{r})} - \frac{1}{\rho(\mathbf{r})} \nabla \int_{(\Delta v)} S_v(\mathbf{r}) dv, \quad (2)$$

where

$$k_v(\mathbf{r}) = h\nu N(\mathbf{r}) B \sum_{j=0}^{\infty} \sum_{\alpha=0}^1 S_{j\alpha}(\mathbf{r}) \Phi_{j\alpha}(\nu, \mathbf{r}),$$

$$B = \frac{2\pi}{3\hbar^2 c} \frac{B_e J_e^2}{\omega_e} \left(\frac{\partial \mu}{\partial r} \right)_{r=r_e}^2,$$

$$\Phi_{j\alpha}(\nu, \mathbf{r}) = \frac{\exp \left\{ - \left(\frac{\nu - \nu_{j\alpha}}{\gamma_{j\alpha}(\mathbf{r})} \right)^2 \right\}}{\pi^{\frac{1}{2}} \gamma_{j\alpha}(\mathbf{r})},$$

$$S_{j\alpha}(\mathbf{r}) = (j + \alpha) \frac{hcB_e}{k_B T(\mathbf{r})} \exp \left\{ - j(j+1) \frac{hcB_e}{k_B T(\mathbf{r})} \right\},$$

$$\gamma_{j\alpha}(\mathbf{r}) = \nu_{j\alpha} \left(\frac{2k_B T(\mathbf{r})}{mc^2} \right)^{\frac{1}{2}}, \quad \nu_{j\alpha} = \nu_0 + 2(1 - 2\alpha)(j + \alpha)cB_e,$$

$$\varepsilon(\mathbf{r}) = \frac{h\nu_0}{m} \left[\exp \left(\frac{h\nu_0}{k_B T_v(\mathbf{r})} \right) - 1 \right]^{-1}, \quad I_v^0(\mathbf{r}) = \frac{2m\nu^2}{c^2\nu_0} \varepsilon(\mathbf{r}).$$

For simplicity in the writing, the time argument in the functions is omitted here.

Integrating (1) with respect to the solid angle results in the relation:

$$\nabla S_v(\mathbf{r}) = 4\pi q \nu^2 k_v(\mathbf{r}) \varepsilon(\mathbf{r}) - k_v(\mathbf{r}) \int_{(4\pi)} I(\mathbf{k}, \mathbf{r}) d\Omega, \quad (3)$$

where according to (1), $I(\mathbf{k}, \mathbf{r})$ has the explicit form

$$I(\mathbf{k}, \mathbf{r}) = \int k_v(\mathbf{r}') I_v^0(\mathbf{r}') \exp \{ -\tau_v(\mathbf{r}, \mathbf{r}') \} ds' + \tilde{I}_v(\mathbf{r}_n, \mathbf{n}) \exp \{ -\tau_v(\mathbf{r}, \mathbf{r}_n) \},$$

$$\tau_v(\mathbf{r}, \mathbf{r}') = \int_0^{|\mathbf{r}-\mathbf{r}'|} k_v(s) ds, \quad q = \frac{2m}{c^2\nu_0}.$$

Substituting (3) into (2) results in an integrodifferential equation for the vibrational energy density [2]

$$\left(\frac{\partial}{\partial t} + \mathbf{v}(\mathbf{r}) \nabla + \frac{1}{\tau(\mathbf{r})} \right) \varepsilon(\mathbf{r}) = \int_{\mathbf{v}} G(\mathbf{r}, \mathbf{r}') \varepsilon(\mathbf{r}') d\mathbf{r}' + \frac{\varepsilon^0(\mathbf{r})}{\tau^0(\mathbf{r})} + \psi(\mathbf{r}), \quad (4)$$

where we have introduced the following notation:

$$G(\mathbf{r}, \mathbf{r}') = \frac{q}{\rho(\mathbf{r})} \int_{(\Delta v)} v^3 k_v(\mathbf{r}) k_v(\mathbf{r}') \frac{\exp\{-\tau_v(\mathbf{r}, \mathbf{r}')\}}{|\mathbf{r} - \mathbf{r}'|^2} dv, \quad (5)$$

$$\psi(\mathbf{r}) = \frac{1}{\rho(\mathbf{r})} \int_{(\Delta v)} dv \int_{(4\pi)} d\Omega k_v(\mathbf{r}) \hat{I}_v(\mathbf{r}, \mathbf{n}) \exp\{-\tau_v(\mathbf{r}, \mathbf{r}_n)\}, \quad (6)$$

$$\frac{1}{\tau(\mathbf{r})} = \frac{1}{\tau^0(\mathbf{r})} + \frac{1}{\tau^*}, \quad \frac{1}{\tau^*} \approx \frac{8\pi h B v_0^3}{c^2}. \quad (7)$$

A sequential quantum-statistical derivation of the equations presented was first given in [2,5-7]. However, let us note that it is convenient to simplify the kernel $G(\mathbf{r}, \mathbf{r}')$ of the fundamental equation of the theory of nonequilibrium diatomic gas radiation transfer (4) for practical computations. Following [2, 7], expression (5) is successfully integrated approximately with respect to the frequency in an arbitrary spatially inhomogeneous case, which results in the expression

$$G(\mathbf{r}, \mathbf{r}') = (hc)^{5/2} \left(\frac{B_e}{m} \right)^{1/2} \frac{\omega_e^3 B^2}{k_B} \frac{\rho(\mathbf{r}') (T(\mathbf{r}) T(\mathbf{r}'))^{1/2}}{(T(\mathbf{r}) + T(\mathbf{r}'))^2} \frac{\exp\left\{ -\frac{\tau_c(\mathbf{r}, \mathbf{r}')}{\sqrt{2}} \right\}}{\sqrt{2} |\mathbf{r} - \mathbf{r}'|^2}, \quad (8)$$

$$\tau_c(\mathbf{r}, \mathbf{r}') = (hc)^{3/2} \left(\frac{B_e}{m} \right)^{1/2} \frac{B}{8k_B} \int_0^{|\mathbf{r} - \mathbf{r}'|} \frac{\rho(s)}{T(s)} ds.$$

In the spatially homogeneous case, the kernel of (8) takes on the especially simple form [8]

$$G(\mathbf{r}, \mathbf{r}') = k \frac{R^*}{4\pi\tau} \frac{\exp\{-k|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|^2}, \quad (9)$$

where

$$k = \frac{\int k_v^2 I_v^0 dv}{\int k_v I_v^0 dv} \approx \frac{(hc)^{3/2}}{8\sqrt{2}} (mB_e)^{1/2} \frac{NB}{k_B T}, \quad (10)$$

$$R^* = \frac{1/\tau^*}{1/\tau^* + 1/\tau^0} = \frac{\tau}{\tau^*}.$$

Here k is the mean absorption coefficient [2, 7], which differs essentially from the corresponding mean coefficients of the equilibrium theory introduced by Planck and Rosseland.

Let us also note that the mean absorption coefficient (10) is useful for calculations of the vibrational energy density distribution $\varepsilon(\mathbf{r})$, while it is not used directly in the calculation of the radiation intensity.

A diffusion approximation [7, 9], which permits obtaining analytical solutions for the vibrational energy density, the spectral intensity, and the radiation flux density, can also be developed in the spatially homogeneous case.

Another case in which an analytical solution is possible is the radiation of optically thin volumes [10].

The need for a computation of the characteristics of multidimensional spatially inhomogeneous volumes of a nonequilibrium gas often occurs in practical applications, however. In mathematical aspects such a problem is no less complex than the problem of computing neutron transport, for whose solution numerical methods, and primarily the Monte Carlo method, are used extensively. The possibility of constructing an effective numerical algorithm for the solution of the fundamental integrodifferential equation (4) also exists for the problem under consideration.

Let us consider the stationary case (velocity, temperature, and pressure fields are independent of the time). The fundamental integrodifferential equation (4) reduces to an integral equation by using Green's function of the transfer operator

$$\left(|v(s)| \frac{d}{ds} + \frac{1}{\tau(s)} \right) D_\gamma(s, s_0) = \delta(s - s_0),$$

$$D_\gamma(s, s_0) = \frac{\phi(s - s_0)}{|v(s_0)|} \exp \left\{ - \int_{s_0}^s \frac{ds'}{\tau(s')|v(s')} \right\}. \quad (11)$$

Here s is the coordinate along the streamline γ and $\phi(s)$ is the Heaviside function. Using (11) the integral equation for $\varepsilon(\mathbf{r})$ has the form

$$\varepsilon(\mathbf{r}) = \lambda \int_V K(\mathbf{r}, \mathbf{r}') \varepsilon(\mathbf{r}') d\mathbf{r}' + \varphi(\mathbf{r}), \quad (12)$$

$$K(\mathbf{r}_1, \mathbf{r}_2) = \int_\gamma D_\gamma(s_1, s) G(\gamma(s), \mathbf{r}_2) ds, \quad (13)$$

$$\varphi(\mathbf{r}_1) = \int_\gamma D_\gamma(s_1, s) \left[\frac{\varepsilon^0(\gamma(s))}{\tau^0(\gamma(s))} + \psi(\gamma(s)) \right] ds, \quad (14)$$

where the streamline $\mathbf{r} = \gamma(s)$ passes through the point $\mathbf{r}_1; \mathbf{r}_1 = \gamma(s_1)$. The parameter $\lambda \leq 1$, whose meaning will become clear later, is introduced formally in (12), but it should tend to one in the final results.

Let us also define the function $U(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N)$:

$$U(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N) = U(\mathbf{r}_0, \mathbf{r}_1) + U(\mathbf{r}_1, \mathbf{r}_2) + \dots + U(\mathbf{r}_{N-1}, \mathbf{r}_N),$$

where $U(\mathbf{r}_i, \mathbf{r}_k) = \ln K(\mathbf{r}_i, \mathbf{r}_k)$; then by iterating the integral equation (12) we obtain

$$\varepsilon(\mathbf{r}_0) = \varphi(\mathbf{r}_0) + \sum_{N=1}^{\infty} \lambda^N \int_V \dots \int_V \exp \{U(\mathbf{r}_0, \dots, \mathbf{r}_N)\} \varphi(\mathbf{r}_N) d\mathbf{r}_1 \dots d\mathbf{r}_N. \quad (15)$$

The Neumann series (15) converges since the norm of kernel (13) is less than one, as is easily shown. The observed radiation characteristics are related in a simple manner to the linear functional $F[\varepsilon]$ of the vibrational energy density $\varepsilon(\mathbf{r})$

$$F[\varepsilon] = \int_V f(\mathbf{r}) \varepsilon(\mathbf{r}) d\mathbf{r} = Q(\lambda) \sum_{N=0}^{\infty} \int_V \dots \int_V \rho(\mathbf{r}_0, \dots, \mathbf{r}_N) f(\mathbf{r}_0) \varphi(\mathbf{r}_N) d\mathbf{r}_0 \dots d\mathbf{r}_N. \quad (16)$$

Here, by following the formal analogy with classical statistical mechanics, quantities of the probability density ρ and partition function Q type are defined for a large canonic ensemble

$$\rho(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N; \lambda) = Q^{-1}(\lambda) \lambda^N \exp \{U(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N)\}, \quad (17)$$

$$Q(\lambda) = \sum_{N=0}^{\infty} \lambda^N \int_V \dots \int_V \exp \{U(\mathbf{r}_0, \dots, \mathbf{r}_N)\} d\mathbf{r}_0 \dots d\mathbf{r}_N, \quad (18)$$

$$\sum_{N=0}^{\infty} \int_V \dots \int_V \rho(\mathbf{r}_0, \dots, \mathbf{r}_N; \lambda) d\mathbf{r}_0 \dots d\mathbf{r}_N = 1, \quad (19)$$

where it is assumed that $U(\mathbf{r}_0) = 0$ everywhere, and therefore $\rho(\mathbf{r}_0) = Q^{-1}(\lambda)$. Let us note that $f(\mathbf{r})$ in (16) is a known function. Thus, e.g., if we are interested in the spectral intensity of the radiation emerging from the volume at a frequency ν along the ray $\mathbf{r}_0 = \mathbf{r}_0(s_0)$, then

$$f(s_0) = q\nu^3 k'_\nu(\mathbf{r}_0) \exp\{-\tau_\nu(\mathbf{r}_0, \mathbf{r}_n)\}, \quad \mathbf{r}_0 = \mathbf{r}_0(s_0), \quad (20)$$

$$I[\varepsilon] = \sum_{N=0}^{\infty} \lambda^N \int_0^l \int_V \dots \int_V \exp\{U(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N)\} f(s_0) \Phi(\mathbf{r}_N) ds_0 d\mathbf{r}_1 \dots d\mathbf{r}_N.$$

In calculating functional (16) it is useful to go over to the integral sums for which we divide the space V into a large number of equal cells with volume v , then (16) and (18) become

$$F[\varepsilon] = Q(\lambda) \sum_{A_i} P(A_i) \Phi(A_i), \quad (21)$$

$$Q(\lambda) = v \sum_{A_i} (\lambda v)^{N_i} \exp\{U(A_i)\}, \quad (22)$$

where $P(A_i)$ is the probability of the states A_i :

$$P(A_i) = \frac{v(\lambda v)^{N_i}}{Q(\lambda)} \exp\{U(A_i)\}, \quad \sum_{A_i} P(A_i) = 1, \quad (23)$$

$$U(A_i) = U(\mathbf{r}_0^{(i)}, \mathbf{r}_1^{(i)}, \dots, \mathbf{r}_{N_i}^{(i)}), \quad \Phi(A_i) = f(\mathbf{r}_0^{(i)}) \Phi(\mathbf{r}_{N_i}^{(i)}).$$

Here A_i denotes the phase-space point of a state with a variable number of particles

$$A_i = (\mathbf{r}_0^{(i)}, \mathbf{r}_1^{(i)}, \dots, \mathbf{r}_{N_i}^{(i)}),$$

where N_i runs through the values 0 to ∞ , and $\mathbf{r}_s^{(i)}$ belongs to the set of the discrete partition cell centers of the volume V at equal elements v . For fixed N there evidently exists $(V/v)^{N_i+1}$ different states A_i .

The probabilistic interpretation of the Neumann series (5) also permits examination of the state A_i as a photon trajectory generated at the point $\mathbf{r}_s^{(i)}$ and experiencing scattering at the sequence of points $\mathbf{r}_{N_i-1}^{(i)}, \mathbf{r}_{N_i-2}^{(i)}, \dots, \mathbf{r}_0^{(i)}$. The mean value of the states function $R(A_i)$ can be used to determine $Q(\lambda)$

$$R(A_i) = \left(\frac{\beta}{V}\right)^{N_i} \exp\{-U(A_i)\}.$$

For any values of the parameter β we find within the limits $0 < \beta < 1$

$$\bar{R}(\lambda) \equiv \sum_{A_i} P(A_i) R(A_i) = VQ^{-1}(\lambda) \sum_{A_i} (\beta\lambda)^{N_i} \left(\frac{v}{V}\right)^{N_i+1} = VQ^{-1}(\lambda) \sum_{N_i=0}^{\infty} (\beta\lambda)^{N_i} = V(1-\beta\lambda)^{-1}Q^{-1}(\lambda). \quad (25)$$

In this case, evaluation of the functional $F[\varepsilon]$ reduces to finding the mean values $\bar{R}(\lambda)$ and $\bar{\Phi}(\lambda)$

$$F[\varepsilon] = \frac{V\bar{\Phi}(\lambda)}{(1-\beta\lambda)\bar{R}(\lambda)}, \quad (26)$$

where

$$\bar{\Phi}(\lambda) = \sum_{A_i} P(A_i) \Phi(A_i).$$

Another method of determining $Q(\lambda)$, which relies essentially on the introduction of the parameter λ , follows from an examination of the differential equation

$$\frac{\partial}{\partial \lambda} \ln Q(\lambda) = \lambda^{-1} Q^{-1}(\lambda) \sum_{A_i} N_i \lambda^{N_i} \exp\{U(A_i)\} v^{N_i+1} = \lambda^{-1} \sum_{A_i} P(A_i) N_i \equiv \lambda^{-1} \bar{N}(\lambda),$$

from which

$$Q(\lambda) = V \exp \left\{ \int_0^\lambda \bar{N}(\lambda') \frac{d\lambda'}{\lambda'} \right\}. \quad (27)$$

Here the boundary condition $Q(0) = V$ was used. Consequently, taking account of (21) and (27), we obtain

$$F[\varepsilon] = V \exp \left\{ \int_0^\lambda \bar{N}(\lambda') \frac{d\lambda'}{\lambda'} \right\} \bar{\Phi}(\lambda). \quad (28)$$

Let us note that although the probabilities $P(A_i)$ are defined completely (23), the direct calculation of the mean values $\bar{R}(\lambda)$, $\bar{\Phi}(\lambda)$, and $\bar{N}(\lambda)$, needed for the computation of $F[\varepsilon]$, is practically impossible because of the excessively large number of points of the states' phase space. This difficulty can be overcome by performing a sufficiently large number of tests of the random variable A_i distributed with probability $P(A_i): A_{i_1}, A_{i_2}, \dots, A_{i_M}$, from which we obtain the mean values of the states functions directly on the basis of the law of large numbers

$$\bar{R}(\lambda) \simeq \frac{1}{M} \sum_{s=1}^M R(A_{i_s}), \quad \bar{\Phi}(\lambda) \simeq \frac{1}{M} \sum_{s=1}^M \Phi(A_{i_s}), \quad \bar{N}(\lambda) \simeq \frac{1}{M} \sum_{s=1}^M N_{i_s}. \quad (29)$$

Here M is sufficiently large, however, considerably less than the total number of phase space points which tend to infinity as $v \rightarrow 0$.

Therefore, (26) and (28) define two methods of evaluating $F[\varepsilon]$, when (29) is taken into account, if the sequence of random variables A_{i_s} is known.

The method of generating the sequence A_{i_s} can be based on the use of the theory of homogeneous Markov chains [11-13]. According to the general theory, we define W_{ik} , the probability of a transition from the state A_i into the state A_k which satisfies the conditions

$$0 \leq W_{ik} < 1, \quad \sum_{A_k} W_{ik} = 1, \quad (30)$$

$$P(A_i) W_{ik} = P(A_k) W_{ki}. \quad (31)$$

Moreover, to satisfy the conditions of the limit theorem [14], it is assumed that any state A_k is attainable from any A_i in a finite number of transitions.

The solution of (30) and (31), which is sufficiently general for the subsequent purposes, has the following form for $N_i \neq 0$ and $A_i \neq A_k$

$$W_{ik} = \left[\sigma \delta_{N_i, N_k} + \left(\frac{1-\sigma}{2} \right) \delta_{N_i, N_k-1} + \left(\frac{1-\sigma}{2} \right) \delta_{N_i, N_k+1} \right] \pi_k w_{ik} \quad (32)$$

and, respectively, for the case $N_i = 0$ and $A_i \neq A_k$

$$W_{ik} = \left[\left(\frac{1+\sigma}{2} \right) \delta_{N_i, N_k} + \left(\frac{1-\sigma}{2} \right) \delta_{N_i, N_k-1} \right] \pi_k w_{ik}. \quad (33)$$

The diagonal elements of the transition matrix W_{ii} are found from the conditions (30). Here σ is a free parameter of the theory $0 < \sigma < 1$; π_k is the probability of the state A_k for a known value $N_k = N$ satisfying the normalization condition

$$\sum_{\substack{A_k \\ (N_k=N)}} \pi_k = 1; \quad (34)$$

and w_{ik} is the conditional transition probability defined by the expression

$$w_{ik} = \frac{(\lambda v)^{N_k} \pi_k^{-1} \exp \{U(A_k)\}}{(\lambda v)^{N_k} \pi_k^{-1} \exp \{U(A_k)\} + (\lambda v)^{N_i} \pi_i^{-1} \exp \{U(A_i)\}}. \quad (35)$$

Solution (32)-(35) written down allows arbitrariness in the choice of π_k with the single constraints $\pi_k > 0$ for any A_k and π_k satisfies the normalization (34). In the simplest case, we can set $\pi_k = n^{-1}(n-1)^{-N_k}$, $n = V/v$. The following version of the selection of π_k is considerably more general and, moreover, more effective

$$\pi_k = \begin{cases} \zeta_1(r_0^{(k)}) \chi(r_1^{(k)} | r_0^{(k)}) \chi(r_2^{(k)} | r_1^{(k)}) \dots \chi(r_{N_k}^{(k)} | r_{N_k-1}^{(k)}), & N_k \geq 1, \\ \zeta_\mu(r_0^{(k)}), & N_k = 0, \end{cases} \quad (36)$$

where $\mu = 1, 2$ for $r_1 \neq r_k$:

$$\chi(r_i | r_k) > 0, \quad \zeta_\mu(r_i) > 0, \\ \chi(r_i | r_i) = 0, \quad \sum_{r_i \in V} \chi(r_i | r_k) = 1, \quad \sum_{r_i \in V} \zeta_\mu(r_i) = 1. \quad (37)$$

Here $\zeta_\mu(r_i)$ and $\chi(r_i | r_k)$ are arbitrary functions satisfying conditions (37). It is easy to see that conditions (37) automatically result in the normalization (34):

$$\sum_{r_0^{(k)} \in V} \sum_{r_1^{(k)} \in V} \dots \sum_{r_{N_k}^{(k)} \in V} \zeta_1(r_0^{(k)}) \chi(r_1^{(k)} | r_0^{(k)}) \chi(r_2^{(k)} | r_1^{(k)}) \dots \chi(r_{N_k}^{(k)} | r_{N_k-1}^{(k)}) = 1.$$

The solution presented for system (30) and (31) allows three kinds of transitions:

- I. transitions without a change in the number of scattering centers ($N_k = N_i$);
- II. transitions with an increase of one in the number of centers ($N_k = N_i + 1$);
- III. transitions with a diminution by one in the number of centers ($N_k = N_i - 1$).

The explicit scheme for constructing the sequence A_{i_s} on the basis of the solution (32)-(37) obtained starts with performing a type of transition from the arbitrarily selected initial state A_i . It is assumed that only transitions of the types I, II, III, which are realized with the probabilities σ , $1/2(1-\sigma)$, $1/2(1-\sigma)$, respectively, are allowed for $N_i \neq 0$, while the transitions of types I and II, which appear with the probabilities $1/2(1+\sigma)$, $1/2(1-\sigma)$, are allowed for $N_i = 0$. Following this, a finite state A_k is performed with probability π_k for the already known value of N_k . A $r_0^{(k)}$ is hence first selected randomly with the probability $\zeta_\mu(r_0^{(k)})$, then an $r_1^{(k)}$ is randomly selected with the conditional probability $\chi(r_1^{(k)} | r_0^{(k)})$, then an $r_2^{(k)}$ is randomly selected with the conditional probability $\chi(r_2^{(k)} | r_1^{(k)})$, etc.

We find the A_k as a result of the random performance with the probability (36), where if it turns out that $A_k = A_i(r_0^{(k)} = r_0^{(i)}, r_1^{(k)} = r_1^{(i)}, \dots, r_{N_k}^{(k)} = r_{N_i}^{(i)})$, we assume that the transition $A_i \rightarrow A_i$ holds. Otherwise ($A_k \neq A_i$), the random variable ξ ; distributed uniformly in the range $0 \leq \xi \leq 1$, is performed, where if $\xi < w_{ik}$, then the transition into the new state $A_i \rightarrow A_k$ is realized, and for $\xi \geq w_{ik}$ we consider that the transition $A_i \rightarrow A_i$ holds and the state A_i is repeated in the sequence A_{i_s} being performed. To determine the next state of the sequence A_{i_s} , the procedure described is repeated starting with a performance of the type of the next transition, etc.

The scheme described for drawing the transitions satisfies the condition of the limit theorem on the attainability of any state A_k from any A_i in a finite number of transitions. Let us now show that the normalization conditions (30) are satisfied for each A_i .

Let $P(\xi \geq w_{ik}) = 1 - w_{ik}$ be the probability of the event $\xi \geq w_{ik}$, then taking account of (32) and (34), we obtain for the case $N_i \neq 0$

$$\begin{aligned} W_{ii} &= \sigma \pi_i + \sigma \sum_{\substack{A_k \\ (A_k \neq A_i, N_i = N_k)}} \pi_k P(\xi \geq w_{ik}) \\ &+ \left(\frac{1-\sigma}{2}\right) \sum_{\substack{A_k \\ (N_k = N_i + 1)}} \pi_k P(\xi \geq w_{ik}) + \left(\frac{1-\sigma}{2}\right) \sum_{\substack{A_k \\ (N_k = N_i - 1)}} \pi_k P(\xi \geq w_{ik}) = \\ &= \sigma \sum_{\substack{A_k \\ (N_i = N_k)}} \pi_k + \left(\frac{1-\sigma}{2}\right) \sum_{\substack{A_k \\ (N_k = N_i + 1)}} \pi_k + \left(\frac{1-\sigma}{2}\right) \sum_{\substack{A_k \\ (N_k = N_i - 1)}} \pi_k - \\ &\quad - \sum_{\substack{A_k \\ (A_k \neq A_i)}} \left[\sigma \delta_{N_i, N_k} + \left(\frac{1-\sigma}{2}\right) \delta_{N_i, N_k - 1} \right. \\ &\quad \left. + \left(\frac{1-\sigma}{2}\right) \delta_{N_i, N_k + 1} \right] \pi_k w_{ik} = 1 - \sum_{\substack{A_k \\ (A_k \neq A_i)}} W_{ik}. \end{aligned}$$

The proof for the case $N_i = 0$ is performed perfectly analogously. There remains to show that the detailed balance conditions (31) are satisfied, which is seen easily by direct substitution of (32), (33), and (35) into (31).

On the basis of the limit theorem [14], the described scheme permits the construction of a stationary sequence A_i (the Markov chain trajectory). Then $F[\varepsilon]$ can be evaluated by means of (26) and (29), or (28) and (29). Let us note that according to the limit theorem, the initial state A_i can be selected arbitrarily; hence, for definiteness it is convenient to perform it with the probability π_i for $N_i = 0$.

We use the remaining arbitrariness in giving π_k so that states yielding a large contribution to $F[\varepsilon]$ would be selected with the highest probability for the sequence A_i being performed. Starting from (21), it follows that the choice of the probability π_k , proportional to the factors $f(\mathbf{r}_0^{(k)}) \varphi(\mathbf{r}_{N_k}^{(k)}) \exp\{U(A_k)\}$ is optimal. This can be achieved most simply by the following selection of the functions $\zeta_\mu(\mathbf{r}_0)$ and $\chi(\mathbf{r}_i | \mathbf{r}_k)$ for $\mathbf{r}_i \neq \mathbf{r}_k$:

$$\begin{aligned} f_1(\mathbf{r}_k) &= f(\mathbf{r}_k), \quad f_2(\mathbf{r}_k) = f(\mathbf{r}_k) \varphi(\mathbf{r}_k), \\ \zeta_\mu(\mathbf{r}_k) &= \frac{f_\mu(\mathbf{r}_k)}{\sum_{\mathbf{r}_s \in V} f_\mu(\mathbf{r}_s)}, \quad \chi(\mathbf{r}_i | \mathbf{r}_k) = \frac{K(\mathbf{r}_k, \mathbf{r}_i) \varphi(\mathbf{r}_i)}{\sum_{\mathbf{r}_s \in V} K(\mathbf{r}_k, \mathbf{r}_s) \varphi(\mathbf{r}_s)}. \end{aligned} \quad (38)$$

Therefore, the determination of π_k by using (36) and (38) permits the efficient calculation of $\bar{\Phi}(\lambda)$, while for the optimal evaluation of $\bar{R}(\lambda)$ or $\bar{N}(\lambda)$ from these same considerations, we should set $f(\mathbf{r}_k) = \varphi(\mathbf{r}_k) = 1$.

Now, when the procedure for calculating the mean values of the states function A_i has been determined, we discuss two methods of determining $Q(\lambda)$ on the basis of (25) and (27). According to (38), the greatest quantity of trajectories is generated in that part of the states space A_i where the probability $P(A_i)$ is relatively large. On the other hand, since the function $R(A_i)$ is inversely proportional to the probability $P(A_i)$, it is clear that the low-probability states, which are relatively small in the sequence A_i being generated, also yield significant contributions to $\bar{R}(\lambda)$. This is why a calculation using (27) is more efficient. The meaning of the introduction of the parameter λ is the realization of this calculation.

Finally, let us turn to the continual limit $\nu \rightarrow 0$, then the positions of the possible photon scattering points are limited only by the volume V itself. For greater definiteness, let us examine the case when the functional $F[\varepsilon]$ is the spectral intensity of the radiation emerging from the volume at a frequency ν along the ray $\mathbf{r}_0 = \mathbf{r}_0(s_0)$. A special consideration is necessary here since in this case function $f(\mathbf{r})$ governing functional (16) is singular. It is convenient to introduce new notations: $A_i = (s_0^{(i)}, \mathbf{r}_1^{(i)}, \mathbf{r}_2^{(i)}, \dots, \mathbf{r}_{N_i}^{(i)})$, $dA_i = ds_0^{(i)} d\mathbf{r}_1^{(i)} d\mathbf{r}_2^{(i)}, \dots, d\mathbf{r}_{N_i}^{(i)}$, then the probability density of the event A_i takes the form

$$\begin{aligned} \bar{P}(A_i) &= \frac{\lambda^{N_i}}{\bar{Q}(\lambda)} \exp \{U(A_i)\}, \quad \sum_{N_i=0}^{\infty} \int_0^l \int_V \dots \int_V \bar{P}(A_i) dA_i = 1, \\ \bar{Q}(\lambda) &= \sum_{N=0}^{\infty} \lambda^N \int_0^l \int_V \dots \int_V \exp \{U(\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_N)\} ds_0 d\mathbf{r}_1 \dots d\mathbf{r}_N. \end{aligned} \quad (39)$$

The spectral intensity of the radiation emerging from the volume is easily obtained in the form

$$I[\varepsilon] = \frac{l\bar{\Phi}(\lambda)}{(1-\beta\lambda)\bar{R}(\lambda)} = l \exp \left\{ \int_0^\lambda \bar{N}(\lambda') \frac{d\lambda'}{\lambda'} \right\} \bar{\Phi}(\lambda), \quad (40)$$

analogously to the derivation of (26) and (28), where l is the geometric path of the ray $\mathbf{r}_0 = \mathbf{r}_0(s_0)$.

Let us note that because of the passage to the limit $\nu \rightarrow 0$, formulas (29) remain valid. Here $\bar{\Phi}(A_i) = f(s_0^{(i)})\varphi(\mathbf{r}_{N_i}^{(i)})$, where $f(s_0)$ is defined by (20).

The transition probability density \bar{w}_{ik} is determined by the substitutions $\pi_k \rightarrow \bar{\pi}_k$ and $w_{ik} \rightarrow \bar{w}_{ik}$ in (32) and (33), where π_k is the probability density of the state A_k for a known N_k

$$\bar{\pi}_k = \begin{cases} \bar{\xi}_1(s_0^{(k)}) \bar{\chi}(\mathbf{r}_1^{(k)} | \mathbf{r}_0^{(k)}) \bar{\chi}(\mathbf{r}_2^{(k)} | \mathbf{r}_1^{(k)}) \dots \bar{\chi}(\mathbf{r}_{N_k}^{(k)} | \mathbf{r}_{N_k-1}^{(k)}), & N_k \geq 1, \\ \bar{\xi}_2(s_0^{(k)}), & N_k = 0, \end{cases} \quad (41)$$

$$\bar{\xi}_\mu(s_0) = \frac{f_\mu(s_0)}{\int_0^l f_\mu(s) ds}, \quad \bar{\chi}(\mathbf{r} | \mathbf{r}') = \frac{K(\mathbf{r}', \mathbf{r}) \varphi(\mathbf{r})}{\int_V K(\mathbf{r}', \mathbf{r}) \varphi(\mathbf{r}) dr}. \quad (42)$$

In this case the normalization condition becomes

$$\int_0^l \int_V \dots \int_V \bar{\pi}_k ds_0^{(k)} d\mathbf{r}_1^{(k)} \dots d\mathbf{r}_{N_k}^{(k)} = 1.$$

The conditional transition probability \bar{w}_{ik} is found by the passage to the limit $\nu \rightarrow 0$ in (35):

$$\bar{w}_{ik} = \frac{\lambda^{N_k} \Pi(A_i)}{\lambda^{N_k} \Pi(A_i) + \lambda^{N_i} \Pi(A_k)}. \quad (43)$$

The following notation is used here $f_1(s_0) = f(s_0)$, $f_2(s_0) = f(s_0)\varphi(\mathbf{r}_0(s_0))$,

$$\Pi(A_k) = \begin{cases} \bar{\xi}_1(s_0^{(k)}) \frac{\varphi(\mathbf{r}_1^{(k)})}{\chi(\mathbf{r}_0^{(k)})} \frac{\varphi(\mathbf{r}_2^{(k)})}{\chi(\mathbf{r}_1^{(k)})} \dots \frac{\varphi(\mathbf{r}_{N_k}^{(k)})}{\chi(\mathbf{r}_{N_k-1}^{(k)})}, & N_k \geq 1, \\ \bar{\xi}_2(s_0^{(k)}), & N_k = 0, \end{cases} \quad (44)$$

$$\mathbf{r}_0^{(k)} = \mathbf{r}_0(s_0^{(k)}), \quad \chi(\mathbf{r}) = \int_V K(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}') dr'. \quad (45)$$

Generation of the trajectory A_{i_s} starts with performance of the type of transition from the arbitrary initial state A_i exactly as in the discrete case described above. The finite state A_k is then performed: First the point $s_0^{(k)}$ is selected randomly on the ray $r_0 = r_0(s_0)$ with the probability density $\tilde{\zeta}_\mu(s_0^{(k)})$, then the point $r_1^{(k)}$ with the conditional probability density $\tilde{\chi}(r_1^{(k)} | r_0^{(k)})$, $r_0^{(k)} = r_0(s_0^{(k)})$, and afterwards the point $r_2^{(k)}$ is selected with the conditional probability density $\tilde{\chi}(r_2^{(k)} | r_1^{(k)})$, etc. Having completed the random selection of the state A_k with the probability density $\tilde{\pi}_k$ in such a manner, the transition $A_i \rightarrow A_k$ itself with probability \tilde{w}_{ik} should be performed. Analogously to the discrete case, if $\xi < \tilde{w}_{ik}$ (ξ is a random variable distributed uniformly in the range $0 \leq \xi \leq 1$), the transition to the new state $A_i \rightarrow A_k$ is realized; otherwise, $A_i \rightarrow A_i^*$. The procedure described is repeated to determine the next state. For definiteness it is convenient to perform the initial state A_i with the density $\tilde{\pi}_i$ at $N_i = 0$. Let us also note that the free parameter of the theory $0 < \sigma < 1$ is defined by the condition of maximal convergence of series (29); in particular, it is possible to set $\sigma = 1/3$. It should be mentioned that a more exact value of the absorption coefficient $k_\nu(r)$ must be used in (20) in the calculation of the spectral radiation intensity than in the integrodifferential equation (4). This is related to the fact that the kernel $G(r, r')$ is an integral quantity in conformity with (5).

The procedure described for finding the Markov chain trajectory is convenient for the evaluation of $\bar{\Phi}(\lambda)$ on the basis of (29). For an effective calculation of $\bar{R}(\lambda)$ or $\bar{N}(\lambda)$, this procedure should be altered somewhat, exactly as in the discrete case, by setting $f(s) = \varphi(r) = 1$ in (41)-(45).

An especially great simplification is possible for optically thin radiating volumes. In this case it is convenient to set $\tilde{\zeta}_\mu(s_0) = 1/V$, $\tilde{\chi}(r|r') = 1/V$ in (41) to find $\bar{\Phi}(\lambda)$, $\bar{R}(\lambda)$, or $\bar{N}(\lambda)$, then we obtain in place of (43)

$$\tilde{w}_{ik} = \frac{(\lambda V)^{N_k} \exp\{U(A_k)\}}{(\lambda V)^{N_k} \exp\{U(A_k)\} + (\lambda V)^{N_i} \exp\{U(A_i)\}}$$

The proposed variation on the Monte Carlo method differs from other methods used in the theory of neutron transport [15, 16] and radiation scattering [17, 18] in that it relies substantially on the theory of homogeneous Markov chains. No less important is the methodological difference associated with normalization on a large ensemble (39) with a variable number of particle scatterings, as well as the numerical realization of the whole procedure (29), (40)-(45).

The approach described affords the possibility of a polynomial approximation in λ for $F[\epsilon]$ with subsequent extrapolation from the domain where the Neumann series converges rapidly $\lambda < 1$, to the desired value $\lambda = 1$. The considered approach is evidently also applicable in the neutron transport theory and the scattering theory for incoherent radiation since the structure of the appropriate equations is analogous to (4) and (12).

NOTATION

$\mathbf{n} = \mathbf{k}/k$, unit vector of photon momentum; $I(\mathbf{k}, \mathbf{r})$, spectral radiation intensity; $I_\nu^0(\mathbf{r})$, source function; \mathbf{k} , wave vector of the electromagnetic radiation; $k_\nu(\mathbf{r})$, absorption coefficient of a diatomic gas at the frequency ν ; $\epsilon(\mathbf{r})$, vibrational energy per unit mass of gas; $\epsilon^0(\mathbf{r})$, equilibrium value of $\epsilon(\mathbf{r})$; $\tau^0(\mathbf{r})$, vibrational relaxation time; $\rho(\mathbf{r})$, mass of gas per unit volume; $S_\nu(\mathbf{r})$, spectral density of the electromagnetic radiation flux; $N(\mathbf{r})$, number of diatomic molecules per unit volume; $V(\mathbf{r})$, mean gas velocity at a point \mathbf{r} ; $\Delta\nu$, vibrational bandwidth; j , rotational quantum number; α , number of the vibrational-rotational branch; $T(\mathbf{r})$, local translational-rotational temperature; $T_\nu(\mathbf{r})$, local vibrational temperature; k_B Boltzmann constant; c , speed of light; m , mass of the diatomic molecule; ν_0 , natural frequency of kernel vibration of a diatomic molecule; B , Einstein coefficient of the stimulated transition $0 \rightarrow 1$; $h = 2\pi\hbar$, Planck's constant; μ , molecule dipole moment; r_e , equilibrium internuclear spacing; $\omega_e = \nu_e/c$, center of the vibrational-rotational band; B_e , rotational constant of the diatomic molecule; $d\Omega$, solid angle differential; $I_\nu(\mathbf{r}, \mathbf{n})$, spectral intensity of the external radiation penetrating through the boundary point \mathbf{r}_n of the volume V in

*As in Russian Original - Publisher.

the direction $\mathbf{n} = \mathbf{k}/k$; τ^* , radiation deactivation time of molecules; k , mean absorption coefficient; R^* , probability of radiation deactivation of the molecules.

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METHODS FOR CALCULATING THE ANISOTROPY OF RADIATION BASED ON AN APPROXIMATION OF THE RADIATION PROPERTIES OF SURFACES

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UDC 536.3

The spatial distribution of radiation is examined in calculating radiation heat transfer between surfaces in a diathermal medium.

Contemporary technological processes require a more detailed study of the spatial distribution of radiation in calculating radiation heat transfer between surfaces in a diathermal medium.

Radiation heat transfer for surfaces with arbitrary emissivities and reflectivities was analyzed very completely in [1] by assuming that the temperature distribution and the optical parameters are given and using the integral equation

$$I_{\text{eff}}(M, s_M) = \varepsilon(M, s_M) I_0(M) + \int_F r(M, s_M, s_{NM}) I_{\text{eff}}(N, s_{NM}) K(M, N) dF_N, \quad (1)$$

where I_{eff} and I_0 are, respectively, the effective and blackbody radiation intensities; \mathbf{s} , direction of emission (reflection); r , brightness coefficient; ε , directional emissivity; $K(M, N) = d\varphi(M, N)/dF_N$, where $d\varphi$ is the elementary angular coefficient and I_{eff} is the quantity sought.

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