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Integrated radiation characteristics with respect to the spectrum are described for the rapid analysis of heat transfer in systems containing hot air with variable temperature and pressure fields.

A new integral method of analyzing the heat transfer by radiation in a real spectrum in the presence of a ruled structure is developed in [1-3]. The method of effective populations [3, 4], based on a great deal of experimental material, is used here to obtain reliable spectrum characteristics, and permits obtaining values of the spectral radiation characteristics that are adequate to the measured values.

Tables of the partial characteristics ΔI (or Som) and ΔSim , intended for flow field and flow divergence analysis in systems of any geometric shape with an arbitrary distribution of the parameters, pressure and temperature, are described in this paper. All the formulas and notation for this case are presented in [5]. The partial intensity ΔI , the source Som and the partial sink ΔSim are computed by means of formulas (1)-(3) from [5].

For systems in which the plane layer approximation can be utilized, the partial characteristics ΔS (or Som) and ΔSim are computed for a plane layer

$$\Delta S(T_{\xi}, P_{\xi}, T_X, P_X, x) = 2 \int_0^{\infty} S_V^0(T_{\xi}) k'_V(T_{\xi}, P_{\xi}) E_2 \left(\int_0^x k'_V(\eta) d\eta \right) dv. \quad (1)$$

$$\text{Som}(T_X, P_X, T_{\xi}, P_{\xi}, x) = 2 \int_0^{\infty} S_V^0(T_X) k'_V(T_X, P_X) E_2 \left(\int_0^x k'_V(\eta) d\eta \right) dv. \quad (2)$$

$$\Delta \text{Sim}(T_{\xi}, P_{\xi}, T_X, P_X, x) = 2 \int_0^{\infty} [S_V^0(T_{\xi}) - S_V^0(T_X)] k'_V(T_{\xi}, P_{\xi}) k'_V(T_X, P_X) E_1 \left(\int_0^x k'_V(\eta) d\eta \right) dv. \quad (3)$$

Here S_V^0 is the unilateral spectral flux, T_{ξ} , P_{ξ} are source parameters (Fig. 1 from [5]), T_X , P_X are parameters of the computation point (or sink), $x = |\xi - X|$ is the geometric distance between the source point ξ and the computation point X . The inner integrals in (1)-(3) are taken over a path given by modeling splines so that the absorption coefficient $k'_V(\eta)$ in these integrals is determined by the distribution of the parameters $T(\eta)$ and $P(\eta)$: $k'_V \equiv k'_V(T_{\eta}, P_{\eta})$. It is seen that the source Som in (2) agrees to the accuracy of the notation, with the partial flux (formula (1)). Therefore, only the two functionals (1) and (3) must be computed. Preliminary results for the case of constant pressure were published by the authors in [6, 7].

Because of their importance, the spectral characteristics of an air plasma were computed by many author collectives [8-10]. Data on the cross sections of elementary radiation processes presented in [8] were taken as the basis for the computation of the partial characteristics in this paper. Data from other papers were used in necessary cases. The influence of partial interaction in the plasma was taken into account by the method in [3, 4]. Diagrams of the nitrogen and oxygen atom terms NI and OI and of their ions NII and OII are shown in Figs. 1-4. The ionizing field intensities are presented [in square brackets] after the notations of the appropriate terms (see [3, 4]). The arrows denote the most important multiplets taken into account in the research (with the exception of transitions with the participation of the f-states).

Photoionization cross sections continued into the long-wave domain were used in the analysis of the continuous atomic plasma spectrum. Real populations of the bound states, obtained by the method of effective populations, were taken into account. The photoionization sections

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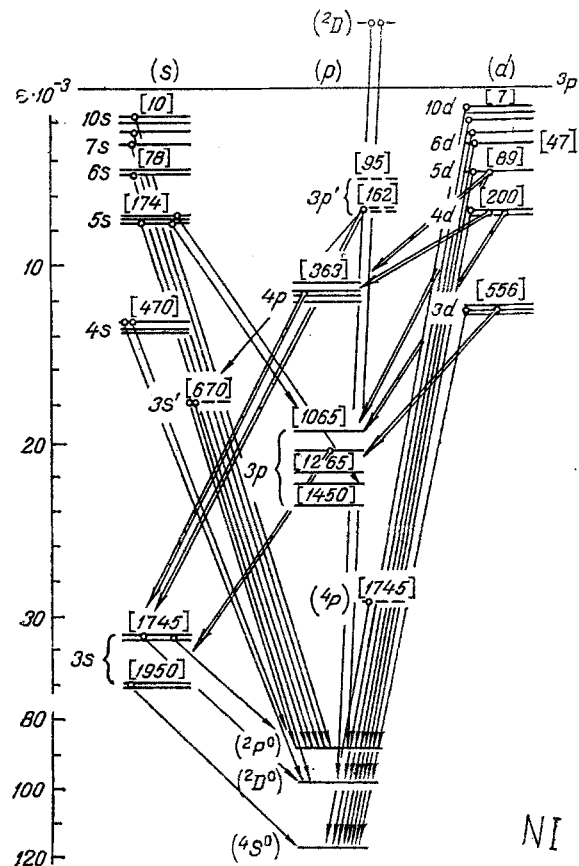


Fig. 1. Diagram of the terms, the ionizing field intensities (kV/cm) and the transitions taken into account for the nitrogen atom, ϵ , cm^{-1} .

were taken from [8, 11-13]. The photostripping of electrons from the negative N^- , O^- , O_2^- ions was taken into account according to [8, 14, 15].

Information about the spectrum line locations, intensities, and halfwidths was taken from [8, 16]. Stark, resonance, van der Waals, and Doppler broadening mechanisms were taken into account. The convolution of all the mechanisms mentioned results in a Voigt profile that was computed by using approximations [17]. All the spectrum series in this paper go over smoothly into the photoionization continuums because of utilization of the method of effective populations. Absorption in the molecular bands O_2 , N_2 , NO , N_2^+ , NO_2 with smoothed out rotational structure was taken into account to temperatures of $14,000^\circ\text{K}$. Photodissociation processes for the molecules O_2 and N_2 and photoionization of the molecule NO were also taken into account. The cross sections of the molecular processes listed were taken from [8]. A computation of the hot air composition is presented in [18].

The optical density τ was calculated by Simpson's rule with an $x/16$ step. The error in the overwhelming majority of the tabulated points did not here exceed 1%. The greatest error of several percent was obtained in a computation in the near ultraviolet range. This error yields a small contribution to the integrated characteristics. Linear interpolation in the temperature T and the logarithm of the pressure P , yielding an error estimated to be 1%, was used in calculating τ for the spectral absorption coefficient k_V^i .

On the order of 1% is introduced into the characteristic by integration over the spectrum line contour using the trapezoid formula. The indeterminacy in the absorption coefficient k_V^i introduces the main error in the computation. This indeterminacy reaches two in individual spectral intervals.

Partial intensities were calculated by bilinear splines (see [1-3, 5]) to confirm the accuracy of the partial characteristics method for an air plasma. The results of computations performed by I. I. Maslennikova showed that stratification of the curves is insignificant with conservation on the spline $\int k_V^i(\eta) d\eta$.

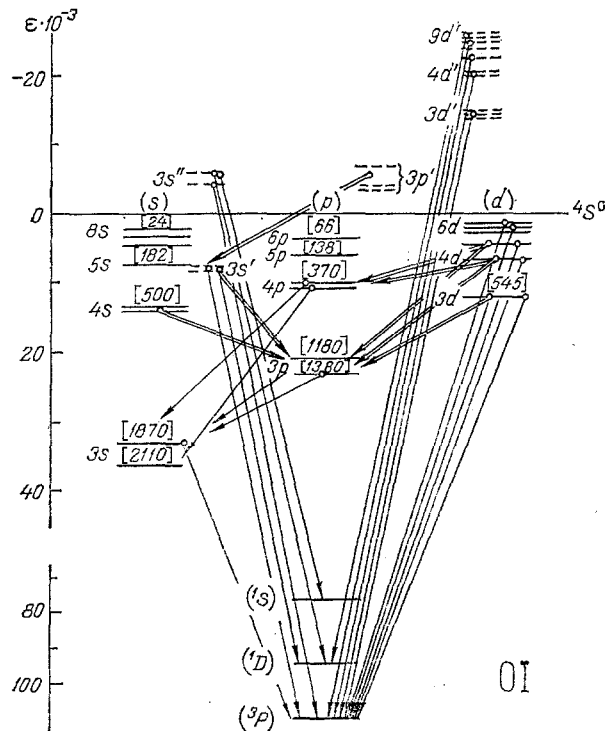


Fig. 2. Diagram of terms, the ionizing field intensities, and the transitions taken into account for the oxygen atom.

The partial characteristics tables being described are intended for computation of the intensity, the radiant energy flux fields, and divergences in systems with characteristic dimension to 1 m that contain hot air, with an arbitrary pressure distribution in the 0.1-30 bar range, and room to 20,000°K temperature range.

The tables have five input parameters (T_ξ , P_ξ , T_X , P_X , x). The source temperature T_ξ is given from 8000 to 20,000°K with a $\Delta T_\xi = 2000^\circ\text{K}$ spacing. The contribution of sections with temperature $T_\xi < 8000^\circ\text{K}$ to the heat transfer is negligible. The temperature of the computation point (or sink) T_X is given from 2000 to 20,000°K with a $\Delta T_X = 2000^\circ\text{K}$ spacing. For points of the volume in which the temperature is $T_X < 2000^\circ\text{K}$, it can be set at 2000°K since the error will be small here.

The scales for the pressure and the geometric dimensions are given in a logarithmic scale. The logarithm of the pressure (P in bar) varies between -1 and $+1.5$, which assures a computation for pressures from 0.1 to 30 bar. The logarithm of x (x in centimeters) varies between -2 and $+2$, which corresponds to dimensions from 0.1 mm to 1 m. The mantissa and the orders are presented in the tables. Thus the number $81 + 01$ corresponds to the quantity $0.81 \cdot 10^1$.

The dimensionalities of the partial characteristics and the results of their integration for an arbitrary geometry have the form: ΔI in $\text{W} \cdot \text{cm}^{-3} \cdot \text{sr}^{-1}$, ΔSim in $\text{W} \cdot \text{cm}^{-4} \cdot \text{sr}^{-1}$, I in $\text{W} \cdot \text{cm}^{-2} \cdot \text{sr}^{-1}$, ∇I in $\text{W} \cdot \text{cm}^{-3} \cdot \text{sr}^{-1}$, S in $\text{W} \cdot \text{cm}^{-2}$, ∇S in $\text{W} \cdot \text{cm}^{-3}$. The dimensionalities of the corresponding quantities for the plane layer model are ΔS in $\text{W} \cdot \text{cm}^{-3}$, ΔSim in $\text{W} \cdot \text{cm}^{-4}$, S in $\text{W} \cdot \text{cm}^{-2}$, ∇S in $\text{W} \cdot \text{cm}^{-3}$.

Radiation fields were computed for known temperature and pressure fields by using the tables described. The intensity in a system with arbitrary geometry was computed by means of formula (4) in [5]. The flux is calculated at a point X (Fig. 1 from [5]) by a single integration in the plane layer model:

$$S(X) = \int_0^L \Delta S(T_\xi, P_\xi, T_X, P_X, x) \text{sign}(\xi - X) d\xi. \quad (4)$$

The parameters T_ξ and P_ξ equal the temperature and pressure at the point ξ and are source parameters while T_X and P_X are the temperature and pressure of the computation point X .

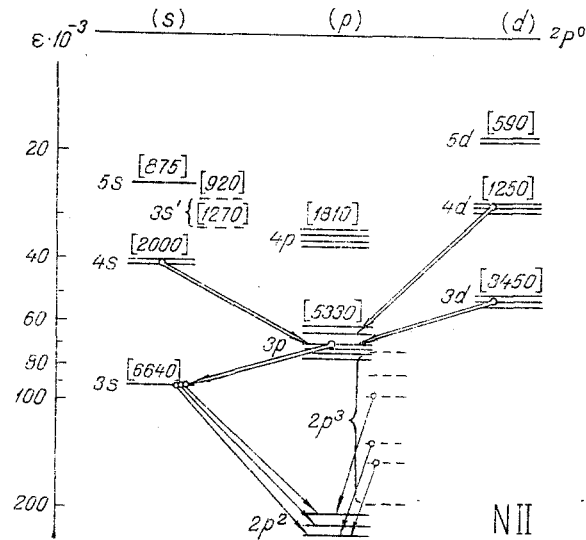


Fig. 3. Diagram of terms, the ionizing field intensities, and the transitions taken into account for the nitrogen ion.

For a rough computation these parameters are taken right at the point X. For a more exact computation, T_X and P_X are determined by means of formulas (5) and (6) from [5]. The integration step $d\xi$ in (4) can be chosen from the existing gasdynamic mesh. There is no necessity to construct a special mesh for the computation of the radiation field by the partial characteristics method. The limit L in the integral (4) is determined by the thickness of the plane layer (Fig. 1 from [5]).

After the intensity field has been computed in the arbitrary geometry case, the flux field can be calculated by means of formula (7) from [5]. To determine the radiation flux divergence in the case of arbitrary geometry, the quantity ∇I must first be computed by means of formula (11) from [5]. The radiation flux divergence in the plane layer model was computed from the single integration

$$\nabla S(X) = \text{Som}(X, 0) + \text{Som}(X, L) - \int_0^L \Delta \text{Sim}(\xi, X) d\xi. \quad (5)$$

Here the first two terms are the effective photo source leaving to the left and the right from the point X (Fig. 1 from [5]) with absorption taken into account on the paths $X \rightarrow 0$ and $X \rightarrow L$.

The sources $\text{Som}(X, 0)$ and $\text{Som}(X, L)$ in (5) are selected from the array ΔS by means of the rule

$$\text{Som}(X, 0) = \Delta S(T_X, P_X, T_0, P_0, x). \quad (6)$$

$$\text{Som}(X, L) = \Delta S(T_X, P_X, T_L, P_L, x). \quad (7)$$

The temperature T_X and pressure P_X at the point X are source parameters in (6) and (7), and consequently are the first pairs of parameters in the matrix $\Delta S(T_1, P_1, T_2, P_2, x)$, i.e., should be substituted into the matrix ΔS in place of the parameters T_ξ and P_ξ . The parameters T_L and P_L in (7), as well as the parameters T_0 and P_0 in (6), are the temperature and pressure of the boundaries of the radiating volume (Fig. 1 from [5]). For an exact computation the parameters T'_L and P'_L it is desirable to compute by means of (13) and (14) from [5], and the parameters T'_0 and P'_0 by analogous formulas

$$T'_0 = \frac{2}{x} \int_0^x T(\eta) d\eta - T_X. \quad (8)$$

$$P'_0 = \frac{2}{x} \int_0^x P(\eta) d\eta - P_X. \quad (9)$$

The parameters T'_L and P'_L in (7) as well as the parameters T'_0 and P'_0 in (6) are the second pair of parameters of the matrix ΔS . The x in (8), (9) as well as in the matrix ΔS when utilizing (6) and (7), equals $x = |L - X|$ or $x = X$.

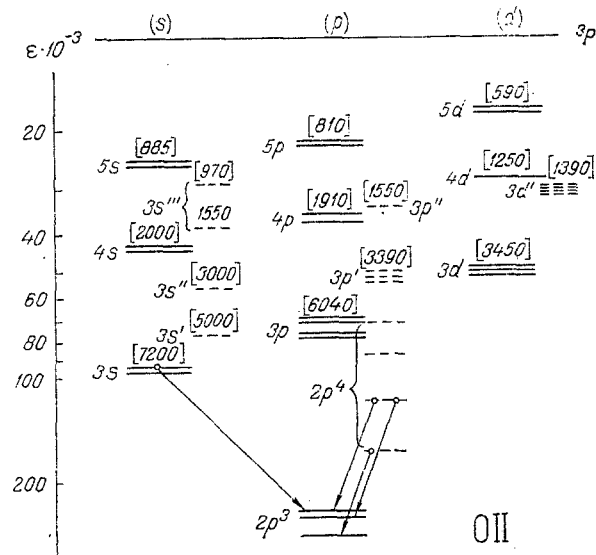


Fig. 4. Diagram of terms, the ionizing field intensities, and the transitions taken into account for the oxygen ion.

The integral in the right side of (5) is an effective sink and is computed by using the matrix of partial sinks $\Delta\text{Sim}(T_{\xi}, P_{\xi}, T_X, P_X, x)$. In this case the parameters T_{ξ}, P_{ξ} of the source and T_X, P_X of the sink points are of identical importance and should be taken right at these points (Fig. 4c from [5]). It should be kept in mind that the matrix ΔSim is antisymmetric relative to simultaneous inversion of the temperature $T_{\xi} \nleftrightarrow T_X$ and pressure $P_{\xi} \nleftrightarrow P_X$ (formula (15) from [5]). Only half the matrix ΔSim is presented for $T_{\xi} > T_X$ in the tables being described. The second half of the matrix (for $T_{\xi} < T_X$) can be stored in the electronic computer memory by using the formula mentioned.

After having computed the quantity ΔI for an arbitrary geometry, the flux divergence is computed by means of formulas (16) and (17) from [5].

The tables described in the paper can be obtained at the Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Academy of Sciences of the USSR (630090, Novosibirsk-90, Institut'skaya, 4/1). The tables can be obtained in the form of the output from an ATSPU (ADC), in the form of punch cards, or inscribed on a magnetic tape of the requestor. The last method is most convenient.

NOTATION

T , absolute temperature; P , pressure; x, X, ξ, η, L , geometric coordinates; k'_ν , absorption coefficient with stimulated emission taken into account; and E_1 and E_2 , exponential integral functions.

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ROTATIONAL EXCITATION OF DIATOMIC MOLECULES IN COLLISIONS

WITH ATOMS

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The rate constants for rotational excitation, the coefficient of RT diffusion for the Ar-N₂ system, and the rotational relaxation time in N₂ are calculated using the quasiclassical approximation.

The growing interest in analytical methods for calculating the rotational excitation of molecules has been aroused by research on the possibilities of creating lasers based on rotational transitions, experiments with expanding jets, studies of the contribution of rotational degrees of freedom to the transport properties of a gas and the behavior of a molecular gas in a magnetic field, research in molecular acoustics, spectroscopy, etc. In [1, 2], a method based on a rigorous quasiclassical approximation to the T scattering operator in terms of action-angle variables was proposed for calculating the vibrational-rotational interaction of particles. In our opinion, this method is more accurate and efficient than previously proposed methods (see, for example, the review in [3]), if we are talking about three-dimensional collisions of complicated objects (polyatomic molecules, clusters) with one another or with a surface. The good accuracy of a simplified variant of this theory (eikonal approximation) achieved in calculations of the differential cross sections of electronic [1] as well as vibrational-rotational [2] excitations with small changes in quantum numbers was demonstrated.

In this work, we continue the investigation of the theory and we perform specific calculations of the rotational excitation of diatomic molecules by atoms using the proposed method for typical gasdynamic conditions. We show that for the model of a plane rotator the increment to the classical action of the atom + rotator system, which determines the transition amplitude, contains only terms that are quadratic with respect to the potential. We include approximately the spatial configurations of the rotator. The cross sections obtained

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