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PROCEDURE OF CALCULATION OF THE OPTICAL CHARACTERISTICS OF SELECTIVELY RADIATING GASES

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The efficiency and correctness of the procedure of calculation of the optical characteristics of selectively radiating and absorbing media proposed by the authors earlier and making it possible to take into account with a high degree of accuracy the fine structure of the absorption line is illustrated with the example of calculation of a number of standard problems of radiative transfer. The reliability of calculation of the absorption coefficient (averaged over a finite spectral interval) of a selective medium is evaluated based on the comparison of the results obtained to the experimental and theoretical data given in the literature.

In designing new high-temperature power plants and technologies and modernizing the existing ones, it is very important to have a preliminary evaluation of the expected results. For this purpose one usually employs the methods of mathematical modeling. In this approach, the accuracy and timeliness of obtaining results largely depend on the correctness and the speed of calculation of the characteristics of radiative transfer. Still greater requirements on programs of calculation of the characteristics of radiation are placed in developing expert diagnostic systems that would make it possible to identify anomalous and emergency situations at an early stage of their genesis based on an analysis of the conditions of radiative heat exchange. In this case, it is especially important to get a result in a real-time regime; therefore, along with ensuring the required accuracy of the solution, great importance is attached to the speed of calculation.

To calculate the characteristics of radiative transfer in selectively radiating and absorbing media it is necessary to solve an integro-differential equation of radiation transfer, which contains an absorption coefficient that describes the selective properties of a medium. Correct account of the selectivity of such a medium can be taken by direct integration of the equation over the contour of the absorption lines. However, this method requires enormous expenditure of computer time since it is necessary to try to select a great number of absorption lines of molecular gases (H_2O, CO_2, CO, etc.). At the same time, additional difficulties occur if in the medium there are particles of the dispersed phase that scatter radiation. An analysis of the literature shows that the approaches to the solution of this problem used at present are inefficient since they are either very labor-consuming [4, 5], or unable to ensure sufficient accuracy of the calculations [6].

An efficient procedure of determination of the absorption coefficient (averaged over a finite spectral interval) of selectively radiating gases with account taken of scattering has been proposed recently in [1–3]; this procedure allows one to avoid integration of the transfer equation with respect to frequency and, in so doing, substantially simplifies the calculation of the characteristics of radiative transfer in selectively radiating, absorbing, and scattering media.

The absorption coefficient (averaged over a finite spectral interval) of a medium is represented in the form of the function

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$$\bar{\chi} = \frac{s}{d}\,\xi\left(\frac{\gamma}{d},\,\tau_a\right)\vartheta\left(\frac{\gamma}{d},\,\tau_a,\,\mathrm{Sc}\right), \tag{1}$$

which depends on the parameters of the absorption line and the Schuster number $\mathrm{Sc} = \sigma/(\chi_p + s/d + \sigma)$ (χ_p is the coefficient of absorption of particles, which is "gray" within the limits of the absorption line). Here $\xi(\gamma/d,\ \tau_a)$ is the correction factor to take into account the contour of the line of radiation in a nonscattering medium ($\mathrm{Sc} = 0$, $\vartheta = 1$), $\vartheta(\gamma/d, \tau_a, \mathrm{Sc})$ is the correction factor to take into account the influence of scattering on the contour of outgoing radiation, and $\tau_a = Hs/d$ is the "gray" optical thickness of the selective component of the medium. If $\chi_p \neq 0$, the absorption coefficient of the medium is determined by the sum $\chi = \bar{\chi} + \chi_p$.

For the Lorentz contour of the absorption line the optical density of the medium with respect to absorption is equal to

$$\tau\,(z) = \tau_a\,\zeta\left(\frac{\gamma}{d},\,z\right), \tag{2}$$

where $\zeta\left(\frac{\gamma}{d}, z\right) = \sinh\left(2\pi\frac{\gamma}{d}\right)\Big/\left[\cosh\left(2\pi\frac{\gamma}{d}\right) - \cos\,(2\pi z)\right]$ is the function that determines the shape of the Lorentz contour of the absorption line [7].

In nonscattering media ($\mathrm{Sc} = 0$), the correction factor $\vartheta\left(\frac{\gamma}{d}, \tau_a, \mathrm{Sc}\right)$ in expression (1) is equal to unity. Therefore, in this case the absorption coefficient (averaged over the line contour) of the selective component will have a simpler form

$$\bar{\chi} = \frac{s}{d}\,\xi\left(\frac{\gamma}{d},\,\tau_a\right), \tag{3}$$

and the value of the correction factor $\xi(\gamma/d, \tau_a)$ to take into account the shape of the absorption line can be determined from an analytical solution of the equation of radiation transfer under the assumption of the absence of external radiation and $B(T)$ = const:

$$\xi\left(\frac{\gamma}{d},\,\tau_a\right) = -\frac{1}{\tau_a}\ln\int_{-0.5}^{0.5}\exp\left(-\tau_a\,\zeta\left(\frac{\gamma}{d},\,z\right)\right)dz\,. \tag{4}$$

This formula can directly be applied to calculations of radiative heat exchange in selective nonscattering media. However, the gain in the counting time will not be great since the process of high-accuracy integration requires significant expenditure of this time. It is expedient to use this formula as a test for evaluating the error of the results obtained using simpler expressions.

The tables of the numerical values of the factor $\xi(\gamma/d, \tau_a)$ which have been calculated from relation (4) for the range of variation of the parameters $10^{-4} < \tau_a \leq 10^4$ and $0.001 \leq \gamma/d \leq 0.5$ are given in [1, 2]. Numerical integration has been carried out according to the Simpson formula accurate to 0.0001%. In these works, the authors have given the approximate formula obtained with the methods of correlation analysis for calculation of the correction factor $\xi(\gamma/d, \tau_a)$:

$$\xi\left(\frac{\gamma}{d},\,\tau\right) = 2\,\frac{\gamma}{d}\left[1 - \exp\left(-\,0.05635\tau\Big/\left(\frac{\gamma}{d}\right)^2\right)\right] + 1\Big/\sqrt{1 + 0.2254\,\tau\,\frac{\gamma}{d}}\ ; \tag{5}$$

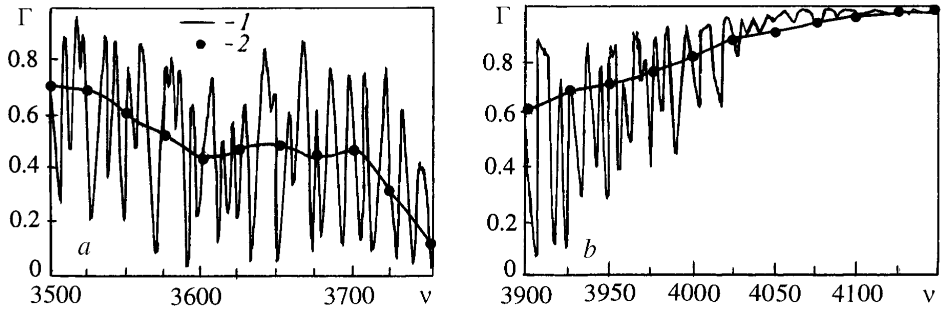

Fig. 1. Transmittance of the vapor of H_2O (steam) (x_{H_2O} = 1): a) P = 0.664 atm, T = 541.9 K, and H = 96.88 mm; b) P = 0.838 atm, T = 672.1 K, and H = 96.36 mm; 1) experiment [8] with a resolution of 0.8 cm^{-1}; 2) calculation from formula (3) with a resolution of 25 cm^{-1}.

in the case where the obtained value of the coefficient turns out to be more than unity one must set $\xi(\gamma/d, \tau_a) = 1$. When formula (5) is used the error of calculation of the radiation intensity does not exceed 4.5% in absolute value throughout the above range of the parameters γ/d and τ_a.

The present work seeks to demonstrate the efficiency and correctness of the procedure proposed in [1] for calculating the optical characteristics of selective gas media. The evaluation of the reliability of the proposed procedure of calculation of the efficient absorption coefficient of a selective medium in a finite spectral interval is illustrated by a comparison of the results obtained in using this procedure to experimental and theoretical data given in the literature. By way of tests we selected standard classical problems that had been used to substantiate the correctness of practically all the existing models of absorption bands: transmission of a layer of homogeneous gas and radiation (emission) of a two-layer gas with different temperature, pressure, and thickness.

It should be noted that the proposed procedure of calculation of the absorption coefficient averaged over the spectral interval is accurate only for a model Lorentz contour of the lines of absorption (radiation). Since the real line contour differs from a model one, the results of the numerical calculations may differ from the real ones. Furthermore, the proposed formula (1) of the absorption coefficient includes the parameters s/d and γ/d determined from the experiment or on the basis of "line by line" calculations; naturally, the accuracy of finding them also affects the error of the calculated value of the absorption coefficient.

At first, let us consider the efficiency of this procedure with the example of calculation of the coefficient of transmission of low-temperature (500–700 K) layers of steam. The results of this calculation obtained from formula (1) and experimentally measured [8] with a resolution of 0.8 cm^{-1} are given in Fig. 1. The thermophysical and geometric parameters of the layers and the spectral resolutions are indicated in the captions to the figures. The values of the average strength of the lines $\bar{s}$ and of the distance between them d in the finite spectral intervals 25 cm^{-1} wide required for the calculation have been taken from tables [9], and the value of the half-width γ of the absorption lines of H_2O in the medium of H_2O has been calculated from the formula [8, 10]

$$\gamma_{H_2O-H_2O} = \gamma_{H_2O-\text{air}}\left(1.2\sqrt{\frac{T_0}{T}} + 7.0\,\frac{T_0}{T}\right) = 0.079\,\frac{P}{P_0}\sqrt{\frac{T_0}{T}}\left(1.2\sqrt{\frac{T_0}{T}} + 7.0\,\frac{T_0}{T}\right),\ \ \text{cm}^{-1}, \qquad (6)$$

where T_0 = 296 K and P_0 = 1 atm.

An analysis of the data given in Fig. 1 shows that the proposed procedure reproduces rather correctly the average coefficient of transmission for the real spectrum of H_2O. The same can also be noted for the CO_2

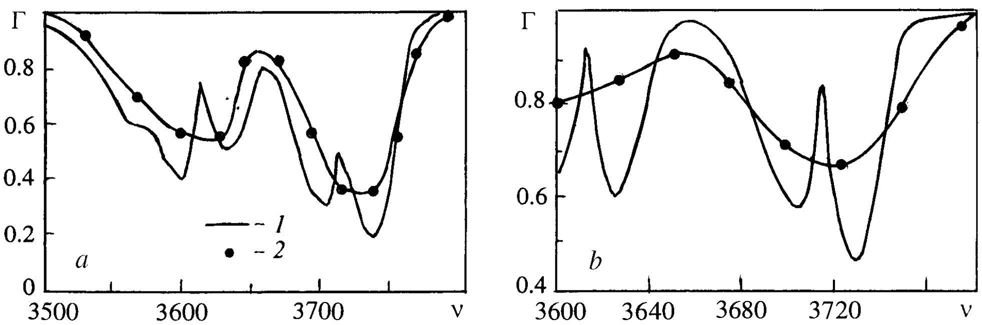

Fig. 2. Transmittance of the vapor of CO_2 in the N_2 medium (x_{CO_2} = 0.155, H = 96.36 mm): a) P = 0.994 atm and T = 291.2 K; b) P = 0.838 atm and T = 672.1 K; 1) experiment [8] with a resolution of 3 cm^{-1}; 2) calculation from formula (3) with a resolution of 25 cm^{-1}.

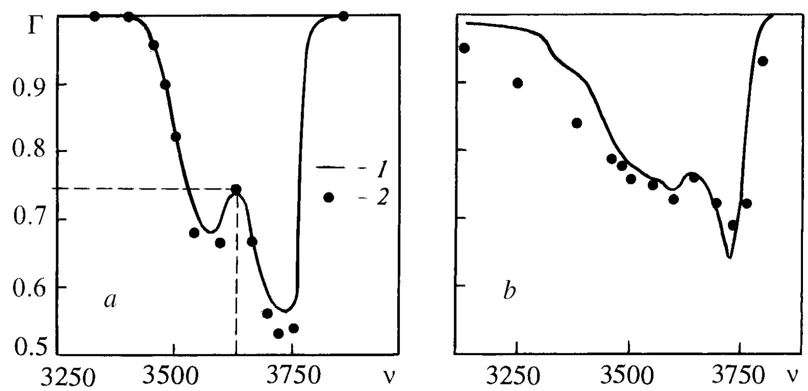

Fig. 3. Transmittance of the layer of CO_2 (x_{CO_2} = 0.05) (a) and of the layer of H_2O (x_{H_2O} = 0.05) (b) in air (P = 1 atm, T = 1000 K, and H = 100 cm) 1) "line by line" calculation [9]; 2) calculation from formula (3) with a resolution of 25 cm^{-1}.

gas in the N_2 medium (Fig. 2), for which the value of the half-width γ of the absorption line of CO_2 has been calculated from the formula [11]

$$\gamma_{CO_2-N_2} = 0.0806 \frac{P}{P_0} \left(\frac{300}{T}\right)^{0.736}, \quad cm^{-1}. \tag{7}$$

Comparison of the numerical results of calculation of the transmittance of the CO_2 and H_2O gases from formula (1) to the data calculated by the accurate "line by line" method [9] also shows their good coincidence (Fig. 3). Although the proposed procedure is an approximate one, it makes it possible to obtain results several hundred thousand times faster than by the "line by line" method.

To demonstrate the simplicity of the use of the procedure proposed, let us calculate the transmittance of CO_2 at a frequency of 3625 cm^{-1} with the parameters given in Fig. 3a.

1. From the tables of [9] we determine the specific value (per atm) of the parameter

$$s/d = 0.0684 \quad cm^{-1} \cdot cm^{-1}.$$

By multiplying this value by the pressure of the gas we obtain the required parameter

$$\frac{s}{d} = P x_{CO_2} \frac{s}{d} = 1 \ \text{atm} \cdot 0.05 \cdot 0.0684 \quad cm^{-1} \cdot atm^{-1} = 0.00342 \quad cm^{-1}.$$

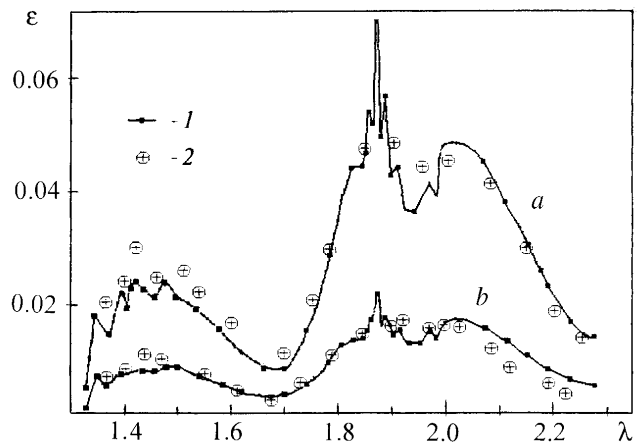

Fig. 4. Spectral emittance of H_2O in air (T = 2900 K, P = 1 atm, x_{H_2O} = 0.58) for the gas layer H = 21.2 (a) and 8 cm (b): 1) experimental data [12]; 2) calculation from formula (3) with a resolution of 25 cm^{-1}.

2. We calculate the "gray" optical thickness

$$\tau_a = \frac{s}{d} H = 0.00342 \ \ \text{cm}^{-1} \cdot 100 \ \ \text{cm} = 0.342 \, .$$

3. From the tables of [9] we determine the parameter $1/d$ = 4.01 cm. The half-width of the absorption line is found from the formula [8]

$$\gamma_{CO_2-\text{air}} = 0.058 \frac{P}{P_0} \left(\frac{T_0}{T} \right)^{0.7} = 0.058 \frac{1}{1} \left(\frac{296}{1000} \right)^{0.7} \approx 0.0274 \, , \ \ \text{cm}^{-1} \, . \tag{8}$$

The required parameter is γ/d = 0.0274 cm^{-1}·4.01 cm ≈ 0.0992.

4. Using the table from [4], we determine the correction factor $\xi(\gamma/d, \tau_a) \approx 0.88$. Then the absorption coefficient is

$$\chi = \xi \frac{s}{d} = 0.88 \cdot 0.00342 \ \ \text{cm}^{-1} \approx 0.00301 \, , \ \ \text{cm}^{-1} \, .$$

5. The transmittance of the gas is calculated from the formula

$$\Gamma = \exp(-\chi H) = \exp(-0.301) \approx 0.74 \, .$$

The indicated value is shown in Fig. 3a as the dashed lines.

As is seen, the procedure of determination of the absorption coefficient (averaged over a finite spectral interval) of a selective component is rather simple and does not require substantial expenditure of computer time while ensuring sufficiently high accuracy of calculation.

Figure 4 gives the comparison of the emittances of a steam $\varepsilon = 1 - \exp(-\chi H)$ in the air medium obtained by experiment [12] and as a result of calculation according to the proposed procedure for different geometric thicknesses of the emitting layer (21.2 and 6.8 cm) within the range of wavelengths λ = 1.8–2.2 mμ. In this case we are dealing with a high-temperature medium heated to T = 2900 K. The partial pressure of the steam was equal to x_{H_2O} = 0.58 atm at a total pressure of the mixture of P = 1 atm. The calculation of the half-width of the lines of absorption of the steam in the air atmosphere was carried out from the formula [10]

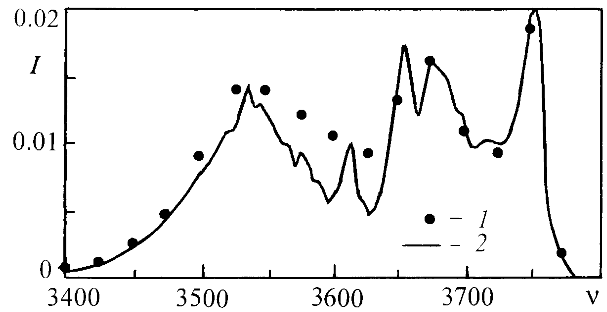

Fig. 5. Spectral intensity of radiation from a hot layer of CO_2 (T_h = 1000 K, H_h = 1 m, x_{CO_2} = 0.03) transmitted by a cold atmosphere consisting of carbon dioxide and nitrogen (T_c = 216 K, H_c = 10 km, x_{CO_2}= 0.0003, P_c = 0.1 atm): 1) "line by line" calculation [10] with a resolution of 5 cm^{-1}; 2) calculation from formula (3) with an averaging of 25 cm^{-1}.

$$\gamma_{H_2O\text{–}air} = 0.079 \frac{P}{P_0} \sqrt{\frac{T_0}{T}} \ , \tag{9}$$

and the parameters of the average strength of the lines $\bar{s}$ and of the distance between them d in finite spectral intervals 25 cm^{-1} wide were selected from the tables of [9]. The results presented in Fig. 4 also confirm the efficiency of the proposed procedure.

In conclusion, let us consider the problem of transmission of the radiation of a hot source by a cold atmosphere and compare the results of the calculations carried out according to the proposed procedure to calculations performed by the "line by line" method [10]. Such problems appear in observing the flares of rockets and airplanes through the atmosphere. The model atmosphere [10] represents a mixture of carbon dioxide and nitrogen at a temperature of 216 K. At an altitude of 10 km, as the rocket is in flight, a 1-m-thick layer of CO_2 (T_h = 1000 K, x_{CO_2} = 0.03, P_h = 0.1 atm) appears. The problem consists of determining the intensity of the emission (radiation) of this layer after its transmission by a cold atmosphere (T_c = 216 K, H_c = 10 km, x_{CO_2} = 0.0003, P_c = 0.1 atm).

The half-width of the absorption lines was determined from formula (8), and the parameters of the average strength of the lines $\bar{s}$ and of the distance between them d in finite spectral intervals 25 cm^{-1} wide required for the calculation were taken from the tables of [9]. The expression for the intensity of radiation on the source side of the cold layer has the form

$$I = B\,(T_h)\,(1 - \exp\,(-\,\chi_h H_h))\,\exp\,(-\,\chi_c H_c) + B\,(T_c)\,(1 - \exp\,(-\,\chi_c H_c))\ , \tag{10}$$

where χ_c and χ_h are the absorption coefficients of the cold and hot layers respectively. The values of the radiation intensity calculated from this formula (the calculation was performed with an averaging of 25 cm^{-1}) are presented in Fig. 5.

The above examples confirm the efficiency of using the procedure proposed in [1–3] for determination of the absorption coefficient (averaged over a finite spectral interval) of a selectively radiating and absorbing gas medium to calculate practical problems of radiative heat exchange.

NOTATION

χ and σ, absorption and scattering coefficients of the medium; $\bar{\chi}$, absorption coefficient of the medium averaged over a finite spectral interval; s, strength of the absorption line; γ, half-width of the absorption line; *d*, distance between the lines; *H*, geometric thickness of the layer; *z*, distance from the center of the line; λ, radiation wavelength; ν, frequency; *T*, temperature; *B*(*T*), Planck function of the temperature; *P*, pressure; *x*, partial pressure; Sc, Schuster number; Γ, transmittance of the gas; ε, emittance of the steam in the air medium. Subscripts: a, averaging over absorption; p, particle; 0, initial value; h, hot; c, cold.

REFERENCES

1. M. L. German, D. Lempert, V. P. Nekrasov, E. F. Nogotov, and S. Rozin, *Inzh.-Fiz. Zh.*, **72**, No. 4, 728–735 (1999).
2. M. L. German, D. Lempert, V. P. Nekrasov, E. F. Nogotov, and S. Rozin, *Inzh.-Fiz. Zh.*, **72**, No. 5, 931–936 (1999).
3. D. Lempert, M. L. German, V. P. Nekrasov, and E. F. Nogotov, in: *Proc. IV Minsk Int. Forum "Heat and Mass Transfer—MIF-2000,"* May 22–26, 2000, Minsk [in Russian], Vol. 2, Minsk (2000), pp. 135–143.
4. C. B. Ludwig, W. Malkmus, and A. L. Thompson, *Handbook on Infrared Radiation from Combustion Gases*, NASA SP-3080, Huntsville, Marshall Space Flight Center (1973).
5. L. S. Rothman, R. R. Gamache, R. H. Tipping, et al., *JQSRT*, **48**, No. 5/6, 469–507 (1992).
6. M. P. Menguc and R. Viskanta, *JQSRT*, **33**, No. 7, 533–541 (1985).
7. V. M. Elsasser, *Phys. Rev*., **54**, No. 2, 126–129 (1938).
8. R. Levi Di Leone and J. Taine, *JQSRT*, **35**, No. 5, 337–343 (1986).
9. A. Soufiani, J. M. Hartmann, and J. Taine, *JQSRT*, **33**, No. 3, 243–257 (1985).
10. L. Pierrot, A. Soufiani, and J. Taine, in: *Proc. 1st Int. Symp. on Radiation Transfer*, Kusadasi, Turkey (1995), pp. 239–250.
11. L. Rosenmann, J. M. Hartmann, M. Perrin, and J. Taine, *Appl. Opt.*, **27**, No. 18, 3902–3907 (1988).
12. A. Coppalle and P. Verlich, *JQSRT*, **35**, No. 2, 121–125 (1986).