RADIATIVE PROPERTIES OF A GAS – SULFER DIOXIDE

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UDC 536.3

An algorithm is initial data are presented for calculating thermal radiation in six bands and the complete spectrum of a gas.

A dioxide is obtained in the combustion of sulfur or sulfur-containing compounds. Estimates of radiative properties obtained up to 1976 were reported in [1]. Using the data obtained by Hottel et al as an example, the authors found that the observations made of emissitivy in the complete spectrum are unreliable. Until now, in engineering calculations it has been necessary to use the parameters of individual bands of the spectrum obtained at or close to room temperature. In the study [2], appearing after [3], specimen temperature was increased to 600 K. Data for higher temperatures (to 2000 K) was extrapolated on the basis of the laws of applied spectroscopy. In contrast to previous investigators, the authors of [2] also considered the weak sixth band of the spectrum. This band had little effect on emissivity, and there was almost no change in the nomograms in [4, 5]. Here, we present algorithms and initial data that can be recommended for heat engineering calculations both in individual bands and in the complete spectrum of the gas.

For a spectrum with nonoverlapping j bands, directional emissivity is calculated from the formula

$$\varepsilon = \frac{\pi}{\sigma T^4} \sum_j I_{0j} \gamma_j \bar{A}_j,$$

where $\pi I_{0j} = \dfrac{37{,}412\,(\omega_j/1000)^3}{\exp(l\omega_j/T) - 1}$; l = 1.4388 cm·K; σ = 5.67·10^{-8} Wt/(m^2·K^4). The quantity $\bar{A}$ is calculated from the Edwards piecewise formulas shown in Table 1, where $\bar{A} = \bar{A}(u; \beta)$, $u = Sx/\gamma$, $\beta = 4b/d$.

The parameters are extrapolated with respect to temperature by means of the approximate formulas

$$S = S_0 (T_0/T)\,\psi,\ \gamma = \gamma_0 \sqrt{T/T_0},$$

$$b/d = P_* \sqrt{T/T_0} C_0^2/(16 S_0 \gamma_0),\ P_* = (B-1)\,p + P.$$

Their error cannot be evaluated; we took B = 1.9. Values of S_0, γ_0 and C_0 at T_0 = 300 K are shown in Table 2. Optical thickness is shown in cm·atm. For the fundamental bands, j = 1, 2, 3, ψ_j = 1. For the next three bands

$$\psi_j = \Phi_j(T)/\Phi(T_0),$$

$$\Phi_4(T) = \frac{1 - \exp[-l(\omega_1 + \omega_3)/T]}{[1 - \exp(-l\omega_1/T)]\,[1 - \exp(-l\omega_3/T)]},$$

$$\Phi_5(T) = \frac{1 - \exp(-2l\omega_1/T)}{[1 - \exp(-l\omega_1/T)]^2},$$

$$\Phi_6(T) = \frac{1 - \exp[-l(\omega_2 + \omega_3)/T]}{[1 - \exp(-l\omega_2/T)]\,[1 - \exp(-l\omega_3/T)]}.$$

The nomogram in [2] is reproduced in accordance with the above-noted algorithm and initial data. It nearly coincides with the nomogram published in [4]. By convention, it is

VNIIENERGOTSVETMET (Sverdlovsk). Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 57, No. 3, pp. 387-391, September, 1989. Original article submitted April 5, 1988.

 0022-0841/89/5703-1016 $12.50

TABLE 1 Calculatio of the Function $\bar{A}(u, \beta_*)$

Formula for $\bar{A}$	β_*	u	
		min	max
u	<1	0	β_*
$2\sqrt{\beta_* u} - \beta_*$		β_*	$1/\beta_*$
$2 - \beta_* + \ln(\beta_* u)$		$1/\beta_*$	∞
u	$\geqslant 1$	0	1
$1 + \ln u$		1	∞

TABLE 2 Parameters of the Spectrum Bonds at T_0 = 300 K

i	Symbol	ω_j cm^{-1}	S_0, (cm^2·atm)$^{-1}$	γ_0, cm^{-1}	C_0, (cm^3·atm)$^{-1/2}$
1	ω_1	1152	113	48	200
2	ω_2	519	110	48	197
3	ω_3	1361	850	20	354
4	$\omega_1+\omega_3$	2500	15,6	32	61
5	$2\omega_1$	2300	2,0	48	27
6	$\omega_2+\omega_2$	1876	4,7	34	34

assumed that the gas is infinitely diluted with nitrogen at normal total pressure, when $P_* = 1$ atm. In any case, a decrease in P_* lowers emissivity – in contrast to the graphs of the corrections for a pure gas in [4, 5].

The formulas in Table 1 have been simplified as much as possible and are approximate. For conventional chambers used in heat-engineering studies.

1. In this case, only the following two formulas are employed:

$$\bar{A} = u \text{ at } u \leqslant 1, \qquad \bar{A} = 1 + \ln u \text{ at } u \geqslant 1. \tag{1}$$

Although it is slight, the effect of pressure on absorption is manifest under all conditions. However, we will assume that it is negligibly small in the present case and will ignore it. The authors of [6] proposed a single formula based on the narrow-band Maier–Goode model with the use of the exponent of the wide-band model

$$\bar{A} = 2E_1(\beta\eta) + E_1(\eta/2) - E_1[\eta(1+2\beta)/2] + \ln[(\beta\eta)^2/(1+2\beta)] + 2\ln\gamma_*, \tag{2}$$

where

$$\eta = \left[\frac{\beta}{u}\left(1 + \frac{\beta}{u}\right)\right]^{-1/2}; \quad \gamma_* = 1.78107.$$

In the present calculations, we used our approximation [7]:

$$E_1(z) = \ln\left[1 + \frac{\gamma_* z + 3.5}{z + 3.5} e^{-z/(\gamma_* z)}\right]$$

with a small error for all z.

Edwards noted in [8, p. 492] that the formulas in Table 1 overestimate the result compared to (2) and similar formulas. However, since the experimental data (including that in [2]) has been analyzed in accordance with these formulas, then the width parameter in (2) should be increased by 20%. Our study confirmed this. Yet the effect of pressure on absorptivity $\bar{A}$ as determined by the parameter β is strong. This contradicts the empirical finding. Arbitrary doubling of the value of β in (2) compared to the calculated value in Table 2 still exaggerates the role of pressure. We will therefore turn to formulas in [9] with a different structure. Their derivation will be described here briefly.

TABLE 3. Calculation of $\bar{A}$

u	$\beta_*=1$	$\beta_*=10$	u	$\beta_*=1$	$\beta_*=10$
0,001	0,001	0,001	10	3,30	3,30
	0,001	0,001		3,49	4,03
	0,000999	0,001		3,45	3,83
0,01	0,01	0,01	100	5,61	5,61
	0,00998	0,00999		5,95	6,10
	0,00998	0,00999		5,63	5,66
0,1	0,1	0,1	1000	7,91	7,91
	0,0981	0,0986		7,41	7,41
	0,0980	0,0985		6,88	6,88
1,0	1,0	1,0			
	0,838	0,873			
	0,833	0,865			

Note. The values in each group from top to bottom correspond to Eqs. (1) and (4) with C = 2.8 and c = 0.03 and Eq. (5) with C = 2.6 and c = 0.015.

In the case of complete overlap of the lines, integral absorption is represented by the wide-band model with a rectangular contour

$$A = \gamma_e[1 - \exp(-Sx/\gamma_e)], \tag{3}$$

where $\gamma_e = \gamma k$; k is a dimensionless parameter reflecting the increase in the width parameter with an increase in optical thickness; $k = C\sqrt{\ln(4.9 + 1.1u)}$. Here, C is correction factor. We obtain

$$\bar{A} = A/\gamma = k[1 - \exp(-u/k)].$$

We allow for the rotational structure within the framework of a statistical narrow-band model in which we make the substitution $u \to w/d$, where w is integral absorption in the line with averaged parameters in the narrow band. In accordance with the Maier–Goode model

$$w/d = (sx/d)/\sqrt{1 + sx/(4b)}.$$

For a rectangular contour, $s/d = S/\gamma$. The formula takes the form

$$\bar{A} = k\left[1 - \exp\left(-\frac{u}{k\sqrt{1 + u/\beta_e}}\right)\right].$$

It includes the rotational structure parameter β_e averaged over the band, this parameter differing from the usual value β. The meaning of transformation (3) is apparent from the fact that an increase in x is a accompanied by an increase in the intensity of the lines at the ends of the band. Due to allowance for this, there is also an increase in the effective width parameter γ_e. However, the effect of pressure on spectral absorptivity remains even in the case of large values of thickness. Thus, the correction for β also depends on thickness. We set $\beta_e = \beta/(ck)$, where c is another correction factor. We finally obtain

$$\bar{A} = k\left[1 - \exp\left(-\frac{u}{k\sqrt{1 + cku/\beta}}\right)\right]. \tag{4}$$

In comparing (4) with the model of a harmonic oscillator and the rigid rotator in [9], we obtained C = 2.22 and c = 0.272. In a unified description of the bands of the spectrum of SO_2 with the use of Eq. (1), we obtained C = 2.8, c = 0.03. The low value of c reflects the weak effect of pressure. The results of calculation of $\bar{A}$ from (1) and (4) are shown in Table 3.

We also tested the Malkmus model [10]. It gives a equally simple formula but is more realistic:

$$w/d = (\beta/2)(\sqrt{1 + 4u/\beta} - 1).$$

With the above correction for the parameter β and some transformation, the final formula takes the form

$$\bar{A} = k\left[1 - \exp\left(-\frac{2u/k}{1 + \sqrt{1 + 4cku/\beta}}\right)\right]. \tag{5}$$

TABLE 4. Comparison of the Emissitivity of SO_2 with Calculation of $\bar{A}$ from (1) (top row) and (5) (bottom row, with C = 2.6 and c = 0.015)

T, K	x=0,03	x=0,12	x=1,2	x=10	x=100
400	0,0126	0,0380	0,167	0,354	0,575
	0,0114	0,0366	0,156	0,380	0,551
600	0,00797	0,0288	0,115	0,288	0,532
	0,00750	0,0257	0,114	0,300	0,526
800	0,00441	0,0175	0,0728	0,208	0,433
	0,00424	0,0152	0,0760	0,211	0,437
1000	0,00250	0,0100	0,0477	0,148	0,338
	0,00243	0,0899	0,0504	0,147	0,347
1200	0,00150	0,00599	0,0324	0,106	0,263
	0,00147	0,00551	0,0339	0,104	0,272
1400	0,000943	0,00377	0,0227	0,0774	0,205
	0,000927	0,00353	0,0234	0,0755	0,213
1600	0,000621	0,00249	0,0165	0,0576	0,162
	0,000613	0,00236	0,0166	0,0563	0,169
2000	0,000301	0,00121	0,00922	0,0339	0,105
	0,000299	0,00116	0,00892	0,0334	0,110

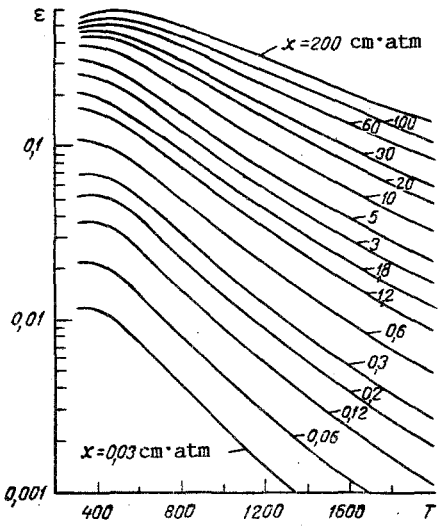

Fig. 1

The results are shown in Table 3 with the following correction factors: C = 2.6 and c = 0.015.

To conclude the analysis, we recommend the use of the data in Table 2 with the additional coefficients in the text. In contrast to the Edwards coefficients in [9], we took n = 1 and B = 1.9 for all six bands.

For conventional heat-engineering equipment, it is recommended that $\bar{A}$ be calculated from Eq. (5) with C = 2.6 and c = 0.015. The difference in the emissivities when $\bar{A}$ is calculated from (1) is shown in Table 4. The nomogram of emissivity was obtained using $\bar{A}$ from (5).

Let us present an estimate of the reliability of the results. The nomogram was limited to 2000 K (see Fig. 1). At higher temperatures, allowance should be made for Doppler broadening and, thus, the Foigt contour of the lines. The same applies to chambers with a highly rarefied medium. The parameters of the bands at room temperature are fairly reliable. However, with an increase in temperature, the spectrum may be enriched by new bands that have not been taken into account. The formulas to extrapolate the parameters with respect to temperature are used only as a first approximation. Their refinement is problematic. Extrapolation with respect to optical thickness is based on experiments conducted only at low temperatures and formulas (1) that have been extremely simplified. One more source of error is the fixing of the centers of the bands. Our studies of the fundamental band of carbon monoxide showed that the center is appreciably dependent on the optical thickness and temperature and that this dependence cannot be described simply. All of the simple models of the broad and

narrow spectral bands will have errors. To solve given problems, it will first of all be necessary to make observations at elevated temperatures for all levels of the spectrum. In the absence of a better method, the present method of calculation is recommended.

To conclude, we will illustrate the use of the method under more general conditions. The density of characteristic radiation at the boundary of a volume of gas with arbitrary fields of temperature, concentration, and pressure is calculated from exact formulas [11]:

$$q_c = \int_{\pi} I \cos\theta d\Omega, \quad I = \frac{\sigma}{\pi} \int_0^{x_0} T^4(x) \frac{\partial a_0 [T(y),\ x]}{\partial x}\bigg|_{y=x} dx,$$

where a_0 is the directional absorptivity of the section x for an incident flow with a black spectrum at the local temperature T(x). The section with the depth x (from the boundary of the volume) is characterized by the parameters $\bar{S}$, $\bar{\gamma}$, and $\bar{\beta}$ averaged from the triparametric approximation [12].

NOTATION

a_0, directional absorptivity of a medium for incident flux with a black spectrum at the temperature T(x); b and d, half-width of the lines and the mean distance between them, cm^{-1}; c, correction factor for the parameter β; k, coefficient expressing the increase in the width parameter, dimensionless; s and S, integral intensities of a line and band, $cm^{-1}/(cm \cdot atm)$; p, P, P_*, partial, total, and effective pressures, atm; x, optical thickness, cm·atm; A, integral absorption in the band, cm^{-1}; $\bar{A} = A/\gamma$; B, line-broadening coefficient, dimensionless; C_0 and C, correction factors for the parameter b/d and k; T, temperature, K; γ, band-width parameter, cm^{-1}; ψ, Φ, functions of the temperature dependence S(T); Ω, solid angle, sr; ε, directional emissivity; ω, wave number, cm^{-1}; $\ell = 1{,}4388$ cm·K; $u = Sx/\gamma$; $\beta = 4$ b/d. Indices: 0 denotes the value at $T_0 = 300$ K.

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