Int. J. Heat Mass Transfer. Vol. 17, pp. 155–158. Pergamon Press 1974. Printed in Great Britain

SHORTER COMMUNICATION

A THEORETICAL CLOSED FORM EXPRESSION FOR THE TOTAL BAND ABSORPTANCE OF INFRARED-RADIATING GASES

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(*Received* 2 *March* 1973 *and in revised form* 18 *June* 1973)

NOMENCLATURE

A,	dimensional band absorptance [cm^{-1}];
$\bar{A}$,	dimensionless band absorptance;
B,	line width to spacing parameter;
C_0,	a constant defined by the band type;
E_1,	first exponential integral;
P_e,	equivalent broadening pressure;
S/d,	mean line intensity to spacing ratio [cm^2 g^{-1}];
u,	dimensionless pathlength;
x,	mass pathlength [g cm^{-2}];
α,	integrated band intensity [cm g^{-1}];
β,	line width to spacing parameter;
γ,	Euler's constant, 0·577216;
η_u,	defined by equation (7);
ν,	wavenumber [cm^{-1}];
τ,	transmissivity;
ω,	band width parameter [cm^{-1}].

1. INTRODUCTION

A VERY useful quantity employed in the calculation of energy transfer from infrared-radiating gases is the total band absorptance. Its importance and its application have been discussed in several recent articles [1–4], and some theoretically and empirically based methods for its determination have been proposed [1, 3, 5–7].

Theoretically, Edwards and Menard [1] proposed the exponential wide band model, and used it in conjunction with the narrow band statistical model to determine the total band absorptance. In their results, and in subsequent modifications, they were only able to define various expressions applicable in different ranges of the governing parameters. Hsieh and Greif [5] using the harmonic oscillator-rigid rotator approximation along with the exponential wide band model calculated the total band absorptance for a variable line intensity Elsasser type band. Their results were only attainable by numerical integration and no general closed form expression was offered. Consequently these theoretical results are only expedient in graphical form.

Other efforts have been directed towards the determination of empirical closed form expressions. Tien and Lowder [6] proposed a fairly accurate, but relatively complex continuous correlation of Edwards' results. Subsequently, Cess and Tiwari [3] offered a simpler but less accurate formula and Tien and Ling [7] proposed a simple two-parameter correlation applicable under certain thermodynamic conditions.

These last three efforts, although producing useful closed form expressions, were empirically based and relied on curve matching techniques for their derivations. The closed form expression offered in the present work, however, is established on a theoretical basis using the identical assumptions which Edwards and Menard originally employed.

2. THEORY

To account for the line structure of a vibration–rotation band the Goody statistical model [8] is used. For a dispersion line shape and an exponential probability distribution, this model predicts the mean spectral transmissivity of a narrow band of rotational lines to be:

$$\tau_\nu = \exp\left\{-\frac{(S/d)\,x}{[1+\{(S/d)x/BP_e\}]^{\frac{1}{2}}}\right\} \tag{1}$$

where (S/d) is the mean line intensity to spacing ratio, B is π times the mean line width to spacing ratio for a dilute mixture at one atmosphere pressure, x is the mass pathlength, P_e an equivalent broadening pressure and ν the wavenumber.

To specify the wavenumber variations of the parameters (S/d) and B, the Edwards model [4] is employed. In this model, it is assumed that B is independent of wavenumber and (S/d) varies only slowly with wavenumber across the entire wide band and not from line to line. This variation is taken to be exponential in nature using the forms:

$$\left(\frac{S}{d}\right)_\nu = \left(\frac{\alpha}{\omega}\right)\exp\left(\frac{-2\,|\nu-\nu_0|}{\omega}\right) \tag{2}$$

for a symmetrical band having a center at ν_0, and:

$$\left(\frac{S}{d}\right)_\nu = \left(\frac{\alpha}{\omega}\right)\exp\left(\frac{-\,|\nu-\nu_0|}{\omega}\right) \tag{2a}$$

for bands with upper or lower wavenumber heads at ν_0. In these expressions α is the integrated band intensity and ω is the band width parameter.

The total band absorptance is defined as:

$$A \equiv \int_{\substack{\text{wide}\\\text{band}}} (1-\tau_\nu)\,d\nu. \tag{3}$$

Upon substituting equations (1) and (2) into (3), the following expression is obtained:

$$A = C_0 \int_0^\infty \left\{ 1 - \exp\left[- \frac{(\alpha/\omega)\, x \exp(-C_0|\nu - \nu_0|/\omega)}{\{1 + [(\alpha/\omega)\, x \exp(-C_0|\nu - \nu_0|/\omega)]/BP_e\}^{\frac{1}{2}}} \right] \right\} \times \mathrm{d}|\nu - \nu_0| \tag{4}$$

where $C_0 = 2$ for a symmetrical band and $C_0 = 1$ for bands with upper or lower wavenumber heads. Letting

$$u = \frac{\alpha}{\omega} x \tag{5}$$

$$\beta = BP_e \tag{6}$$

$$\rho = \left[1 + \frac{u \exp(-C_0|\nu - \nu_0|/\omega)}{\beta} \right]^{\frac{1}{2}}$$

then

$$\mathrm{d}|\nu - \nu_0| = -\frac{2\omega}{C_0} \frac{1}{[(\rho^2 - 1)/\rho]} \mathrm{d}\rho$$

and

$$A = \int_1^{[1+(u/\beta)]^{1/2}} \left\{ 1 - \exp\left[- \frac{\beta(\rho^2 - 1)}{\rho} \right] \frac{2\omega}{[(\rho^2 - 1)/\rho]} \right\} \mathrm{d}\rho.$$

Letting

$$\eta = \left(\frac{\rho^2 - 1}{\rho} \right)$$

then

$$\rho = \frac{\eta \pm \sqrt{(\eta^2 + 4)}}{2}.$$

Since $\rho > 0$ always, the positive root in the above expression must always be taken. Therefore,

$$\rho = \frac{\eta + \sqrt{(\eta^2 + 4)}}{2}$$

and

$$\mathrm{d}\rho = \tfrac{1}{2}\left[1 + \frac{\eta}{\sqrt{(\eta^2 + 4)}} \right] \mathrm{d}\eta.$$

The limits become

$$\rho = 1, \qquad \eta_l = 0$$
$$\rho = \left[1 + \frac{u}{\beta} \right]^{\frac{1}{2}}, \qquad \eta_u = \left[\frac{\beta}{u}\left(1 + \frac{\beta}{u} \right) \right]^{-\frac{1}{2}}. \tag{7}$$

Substituting,

$$A = \omega \int_0^{\eta_u} [1 - \mathrm{e}^{-\beta\eta}] \left(\frac{1}{\eta} \right) \left[1 + \frac{\eta}{(\eta^2 + 4)^{\frac{1}{2}}} \right] \mathrm{d}\eta.$$

Letting

$$\bar{A} = \frac{A}{\omega}$$

$$\xi = \frac{\eta}{\eta_u}$$

there results:

$$\bar{A} = \int_0^1 \frac{(1 - \mathrm{e}^{-\beta\eta_u\xi})}{\xi} \mathrm{d}\xi + \int_0^1 \frac{(1 - \mathrm{e}^{-\beta\eta_u\xi})}{[\xi^2 + (2/\eta_u)^2]^{\frac{1}{2}}} \mathrm{d}\xi. \tag{8}$$

The first integral is given in Abramowitz and Stegun [9] as

$$\int_0^1 \frac{(1 - \mathrm{e}^{-\beta\eta_u\xi})}{\xi} \mathrm{d}\xi = E_1(\beta\eta_u) + \ln(\beta\eta_u) + \gamma \tag{9}$$

where E_1 is the first exponential integral and $\gamma = 0{\cdot}577216$ is Euler's constant. The second integral cannot be directly integrated into a closed form. However, it may be evaluated exactly by numerical integration. In addition, an extremely successful kernel substitution has been discovered that allows the determination of an accurate and relatively simple closed form expression for this integral. The following substitution method yields values that are nearly identical with those of the exact integration.

The substitute kernel is taken to be:

$$\frac{1 - \mathrm{e}^{-x}}{x} \simeq \frac{1}{[x^2 + 1]^{\frac{1}{2}}}. \tag{10}$$

These two expressions are identical in the limits of small and large values of x. That is, for $x \ll 1$ they both approach to one and for $x \gg 1$ they both reduce to $1/x$. Deviation between the two is essentially limited to the range $0{\cdot}2 < x < 2{\cdot}0$ with the maximum difference being 11·5 per cent at about $x = 0{\cdot}8$. Using this substitution, the second integral is evaluated forthright as follows:

letting

$$x = \frac{\eta_u\xi}{2}$$

then

$$\int_0^1 \frac{(1 - \mathrm{e}^{-\beta\eta_u\xi})}{[\xi^2 + (2/\eta_u)^2]^{\frac{1}{2}}} \mathrm{d}\zeta = \int_0^{\eta_u/2} \frac{(1 - \mathrm{e}^{-2\beta x})}{(x^2 + 1)^{\frac{1}{2}}} \mathrm{d}x$$

$$\simeq \int_0^{\eta_u/2} \frac{(1 - \mathrm{e}^{-2\beta x})(1 - \mathrm{e}^{-x})}{x} \mathrm{d}x$$

$$= \int_0^{\eta_u/2} \frac{(1 - \mathrm{e}^{-x})}{x} \mathrm{d}x + \int_0^{\beta\eta_u} \frac{(1 - \mathrm{e}^{-x})}{x} \mathrm{d}x - \int_0^{\eta_u/2\,(1+2\beta)} \frac{(1 - \mathrm{e}^{-x})}{x} \mathrm{d}x$$

$$= [E_1(\eta_u/2) + \ln(\eta_u/2) + \gamma] + [E_1(\beta\eta_u) + \ln(\beta\eta_u) + \gamma] - \{E_1[(\eta_u/2)(1 + 2\beta)] + \ln[(\eta_u/2)(1 + 2\beta)] + \gamma\}.$$

The resulting closed form expression for the total band absorptance is then:

$$\bar{A} = 2E_1(\beta\eta_u) + E_1\left(\frac{\eta_u}{2}\right) - E_1\left[\frac{\eta_u}{2}(1 + 2\beta)\right] + \ln\left[\frac{(\beta\eta_u)^2}{1 + 2\beta}\right] + 2\gamma. \qquad (12)$$

A comparison of the values of $\bar{A}$ as calculated numerically using the exact expression, equation (8), and the closed form expression resulting from the kernel substitution, equation (12), is given in Table 1. The two methods of calculation yield values which are in excellent agreement over the complete range of the governing parameters. Hence, equation (12) may be considered a near exact expression for the total band absorptance.

3. RESULTS AND DISCUSSION

The present results are plotted in Fig. 1 along with the calculations of Hsieh and Greif [5] and the correlation of Tien and Lowder [6]. There is good agreement with the theoretical values of Hsieh and Greif over the entire range of u and β. The Tien–Lowder empirical correlation agrees with the two theoretical methods for values of β on the order of 0·01 and greater, but it appears to be unreliable for values of β smaller than this.

It would be interesting to compare Edwards' four region expressions with the corresponding expressions resulting from the present analysis. Unfortunately, due to the forms of the expansions of the E_1 function the present results cannot be put into expressions which allow comparisons with each of the four Edwards expressions. However, it is possible to make such comparisons in the linear and the "strong" logarithmic regions. The functions for these regions, as defined by Edwards and by equations (8) and (12), are presented in Table 2. As expected, in the linear region the expressions are the same. In the "strong" logarithmic region ($\beta \rightarrow \infty$ and u on the order of 3 or larger) the expressions resulting from equations (8) and (12) are identical whereas Edwards' expression shows the same functional dependence on u but contains a different additive constant. It should be noted that for small to moderate values of u the percentage difference between the expressions can be quite substantial.

Table 1. Comparison of exact and kernel substitution evaluations of the total band absorptance (A_E and A_K respectively)

u \ β	0·001		0·01		0·1		1		10	
	A_E	A_K	A_E	A_K	A_E	A_K	A_E	A_K	A_E	A_K
0·001	0·00083	0·00082	0·00098	0·00098	0·00100	0·00100	0·00100	0·00100	0·00100	0·00100
0·01	0·00463	0·00447	0·00827	0·00817	0·00974	0·00973	0·00995	0·00995	0·00997	0·00997
0·1	0·01805	0·01785	0·04596	0·04487	0·08133	0·08037	0·09532	0·09529	0·09732	0·09732
1	0·06078	0·06072	0·17633	0·17436	0·42780	0·41314	0·69668	0·68897	0·78383	0·78383
10	0·19312	0·19312	0·56642	0·56570	1·4227	1·4046	2·4633	2·3876	2·8300	2·8090
100	0·58378	0·58377	1·5737	1·5733	3·3064	3·2950	4·7418	4·6510	5·1325	5·0213
1000	1·5912	1·5912	3·4588	3·4585	5·5877	5·5772	7·0444	6·9626	7·4351	7·3103
10000	3·4763	3·4763	5·7401	5·7398	7·8903	7·8799	9·3470	9·2661	9·7377	9·6218

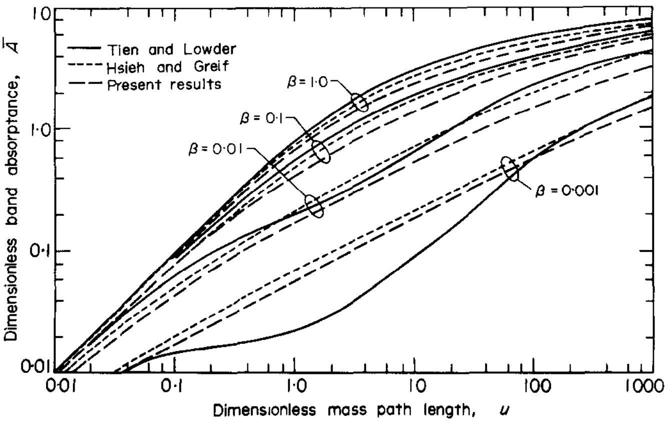

FIG. 1.

Table 2. Comparison of the limiting expressions for the total band absorptance

Basis / Region	Edwards	Equation (12)	Equation (8)
linear	u	u	u
"Strong" logarithmic	$\ln u + 1{\cdot}0$	$\ln u + 0{\cdot}577$	$\ln u + 0{\cdot}577$

Acknowledgement—This research was supported by the National Science Foundation in the Fire Research Program, Research Applied to National Needs (RANN), through Grant GI-43.

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