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A wide-band absorption coefficient integration kernel

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Abstract—The concept of a wide-band absorption coefficient integration kernel is introduced and developed for use in problems involving the radiant heat transfer of real absorbing/emitting gases. For each of the non-transparent, absorption/emission bands of a gas, the kernel transforms the detailed wavenumber integrations to more convenient integrations over the absorption coefficient. A simple expression for the integration kernel is developed from the Tien and Lowder expression for the total band absorptance. The use of the kernel is then illustrated and compared with an exact solution through the example of an isothermal gas between two infinite, parallel plates.

1. INTRODUCTION

For absorbing/emitting gases, it is well known that the spectral absorption coefficient, κ_ν, is a complex irregular function of wavenumber, ν, which greatly complicates calculations of radiative transfer. An attractive alternative to either line-by-line or narrow-band methods of calculation are formulations based upon wide-band absorptance models [1–4]. A characteristic of wide-band model methods is the necessity to formulate the equations of transfer in such a manner that the total band absorptance appears explicitly; see, for example, Tsai and Chan [5]. It is the purpose of this paper to present a technique that allows the available empirical results from wide-band absorption research to be used without such formulations. This is accomplished through the development of a wide-band absorption integration kernel which replaces detailed spectral integrations with a more convenient integration over the absorption coefficient. Our wide-band integration kernel is an extension of the concept of the absorption coefficient distribution function which was developed for use over narrow bands [6, 7].

2. THE WIDE-BAND ABSORPTION COEFFICIENT DISTRIBUTION FUNCTION

For a narrow band, $\delta\nu_i$, Arking and Grossman [6] showed that the integration of a quantity $g(\kappa_\nu)$ over ν may be transformed into an integration over the absorption coefficient, κ, through the use of an absorption coefficient distribution function, $f_i(\kappa)$

$$\frac{1}{\delta\nu_i}\int_{\delta\nu_i} g(\kappa_\nu)\,\mathrm{d}\nu = \int_0^\infty g(\kappa) f_i(\kappa)\,\mathrm{d}\kappa. \tag{1}$$

Arking and Grossman showed that it is only the distribution of κ-values within the band, not the ordering, which determines transmission. Domoto [7] showed that the distribution function is a property of the gas and can be obtained, without explicit knowledge of the absorption coefficient, as the inverse Laplace transform of the transmission function, $T_i(s)$, that is

$$T_i(s) = \int_0^\infty \mathrm{e}^{-\kappa_\nu s} f_i(\kappa)\,\mathrm{d}\kappa \tag{2}$$

$$f_i(\kappa) = L^{-1}[T_i(s)]. \tag{3}$$

Using equation (3), Domoto derived $f_i(\kappa)$ for a number of special cases. In particular, use of the Malkmus model [8] gives

$$f_i(\kappa) = \sqrt{\frac{S_i\beta_i}{4\pi\kappa^3}}\exp\left[\frac{\beta_i}{4}\left(2 - \frac{\kappa}{S_i} - \frac{S_i}{\kappa}\right)\right] \tag{4}$$

where S_i and β_i are the mean line intensity to spacing ratio and the line width to spacing parameter, respectively, for the ith narrow band.

The wavenumber integration of any function $g(\kappa_\nu)$ over a wide-band interval may be obtained as the sum of integrals over the narrow-band intervals:

$$\int_{\Delta\nu} g(\kappa_\nu)\,\mathrm{d}\nu = \sum_i \int_{\delta\nu_i} g(\kappa_\nu)\,\mathrm{d}\nu. \tag{5}$$

Thus, the wide-band integral of $g(\kappa)$ is

$$\int_{\Delta\nu} g(\kappa_\nu)\,\mathrm{d}\nu = \sum_i \delta\nu_i \int_0^\infty g(\kappa) f_i(\kappa_i, S_i, \beta_i)\,\mathrm{d}\kappa. \tag{6}$$

The narrow-band parameters, S_i and β_i, in this equation can vary widely with wavenumber over the wide-band interval. If reasonably smooth variations can be assumed a wide-band distribution function can be developed, as will be shown below.

Several 'wide-band' models of the variation of S_i and β_i with ν across the total band have been

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NOMENCLATURE

A	total band absorptance
a_1	constant in the approximate $H(\kappa)$ function, defined by equation (28a)
a_2	constant in the approximate $H(\kappa)$ function, defined by equation (28b)
a_3	constant in the approximate $H(\kappa)$ function, defined by equation (28c)
c	constant in the Tien and Lowder total band absorptance expression
c_0	constant in the Edwards and Menard exponential model
E_n	exponential integral
e_{bv}	blackbody emissive power
$F(\kappa)$	wide-band distribution function, defined in equation (11)
f_i	narrow-band distribution function, equation (1)
f_2	Tien and Lowder function, equation (25)
$H(\kappa)$	wide-band integration kernel defined in equation (15)
I	intensity of radiation
$P(S)$	S-distribution function defined in equation (9)
q	radiant flux vector
S	mean line intensity to spacing ratio
s	mass path length between absorbing/emitting elements
T_i	narrow band transmission function.

Greek symbols

α	integrated band intensity parameter
α_v	gas absorptance
β	line width to spacing parameter
ε	surface emissivity
κ	absorption coefficient
v	wavenumber
ω	band width parameter.

Subscripts

b	property of a blackbody
g	property of an isothermal gas
v	spectral quantity.

developed [1–4]. One of the simplest is the exponential wide-band model formulated by Edwards and Menard [9] while developing their expressions for correlating the total band absorptance. In this model, the line spacing, and thus the β_i, are assumed to be constant across the band. In addition, the S_i are 're-ordered' within the band and the reordered array of S values is approximated by the smooth exponential function

$$S = \frac{\alpha}{\omega}\exp\left(-\frac{c_0|v-v_0|}{\omega}\right) \tag{7}$$

where α is the integrated band intensity, $\alpha = \int_0^\infty S\,\mathrm{d}(v-v_0)$; ω is the band width parameter; v_0 is the wavenumber at the center of the band; and $c_0 = 1$ for bands with upper or lower wavenumber heads and $c_0 = 2$ for symmetric bands.

Using the exponential band model, equation (6) may be written as

$$\int_{\Delta v} g(\kappa_v)\,\mathrm{d}v = \int_{\Delta v}\int_0^\infty g(\kappa) f(\kappa, S_v, \beta_v)\,\mathrm{d}\kappa\,\mathrm{d}v$$

$$= \Delta v \int_0^\infty \int_0^\infty g(\kappa) f P(S)\,\mathrm{d}\kappa\,\mathrm{d}S \tag{8}$$

where the S-distribution function $P(S)$ represents the frequency of occurrence of S within the wide-band, that is,

$$P(S) \equiv \frac{1}{\Delta v}\left|\frac{\mathrm{d}v}{\mathrm{d}S}\right|. \tag{9}$$

If it is assumed that there exists a definite maximum band width, $\Delta v = c_0|v-v_0|$, at which a corresponding minimum of S occurs, i.e.

$$S_{\min} = \frac{\alpha}{\omega}\mathrm{e}^{-\Delta v/\omega}$$

then, the S-distribution function for the exponential model is given by

$$P(S) = \begin{cases} \dfrac{\omega}{S\Delta v} & S_{\min} \leqslant S \leqslant \alpha/\omega \\ 0 & S < S_{\min},\ S > \alpha/\omega. \end{cases} \tag{10}$$

A wide-band κ-distribution function, $F(\kappa)$, can now be defined as

$$F(\kappa) \equiv \int_0^\infty f(\kappa, S, \beta) P(S)\,\mathrm{d}S. \tag{11}$$

Note from this equation that $F(\kappa)$ can be interpreted as the mean value of f_i over the wide-band interval. The wavenumber integration of the function $g(\kappa_v)$ over the wide band becomes, using equation (11),

$$\int_{\Delta v} g(\kappa_v)\,\mathrm{d}v = \Delta v \int_0^\infty g(\kappa) F(\kappa)\,\mathrm{d}\kappa. \tag{12}$$

An expression for a theoretical wide-band absorption coefficient distribution function can be obtained using equation (11) in conjunction with the exponential wide-band model of S and β and the Malkmus model of the narrow-band distribution function,

equation (4). Thus

$$F(\kappa)=\frac{\omega}{2\kappa\Delta v}\left\{\operatorname{erf}\left[\sqrt{\frac{\beta}{4}}\left(\frac{1}{\sqrt{\bar\kappa}}-\sqrt{\bar\kappa}\right)\right]-\operatorname{erf}\left[\sqrt{\frac{\beta}{4}}\left(\sqrt{\frac{S_{\min}}{\kappa}}-\sqrt{\frac{\kappa}{S_{\min}}}\right)\right]+e^{\beta}\left[\operatorname{erf}\left[\sqrt{\frac{\beta}{4}}\left(\frac{1}{\sqrt{\bar\kappa}}+\sqrt{\bar\kappa}\right)\right]-\operatorname{erf}\left[\sqrt{\frac{\beta}{4}}\left(\sqrt{\frac{S_{\min}}{\kappa}}+\sqrt{\frac{\kappa}{S_{\min}}}\right)\right]\right]\right\} \quad (13)$$

where $\bar\kappa=\omega\kappa/\alpha$.

Use of equation (13) for wavenumber integrations requires specification not only of the wide-band parameters α, β and ω but also of a definite band width, $\Delta\nu$, or $S_{\min}$. In general, the band width depends upon the system geometry or path length. However, if the general function $g(\kappa)$ is constrained such that

$$g(\kappa)\text{ is continuous in }\kappa;\quad g(0)=0 \quad (14)$$

the required wide-band integration is given by

$$\int_{\Delta\nu}g(\kappa_\nu)\,d\nu=\int_0^\infty g(\kappa)H(\kappa)\,d\kappa \quad (15)$$

where the wide-band integration kernel is given by

$$H(\kappa)=\lim_{S_{\min}\to 0}\Delta\nu F(\kappa) \quad (16)$$

$$H(\kappa)=\frac{\omega}{2\kappa}\left\{\operatorname{erfc}\left[\sqrt{\frac{\beta}{4}}\left(\sqrt{\bar\kappa}-\sqrt{\frac{1}{\bar\kappa}}\right)\right]-e^{\beta}\operatorname{erfc}\left[\sqrt{\frac{\beta}{4}}\left(\sqrt{\bar\kappa}+\sqrt{\frac{1}{\bar\kappa}}\right)\right]\right\}. \quad (17)$$

A simple device that guarantees condition (14) is the breaking up of spectral integrals into 'transparent' and 'band' integrals. For example, the wavenumber integration of a general spectral function $G(I_\nu,\kappa_\nu)$ in which the wavenumber dependence comes through both the spectral intensity and the absorption coefficient may be written as

$$\int_0^\infty G_\nu\,d\nu=\int_0^\infty G'_\nu\,d\nu-\int_0^\infty[G'_\nu-G_\nu]\,d\nu \quad (18)$$

where

$$G'_\nu\equiv G_\nu(I_\nu,\kappa_\nu)\quad\text{at }\kappa_\nu=0. \quad (19)$$

The bracketed term $[G'_\nu-G_\nu]$ is identically zero outside the band regions and, assuming that it is also continuous in κ, meets condition (14). Therefore

$$\int_0^\infty G_\nu\,d\nu=\int_0^\infty G'_\nu\,d\nu-\sum_{j\text{ bands}}\int_0^\infty[G'_{\nu_j}-G_{\nu_j}]H_j(\kappa)\,d\kappa. \quad (20)$$

3. APPROXIMATE WIDE-BAND FUNCTION

The wide-band integration kernel described in the previous section is a very complex expression in itself and its use for integrations of even simple functions can be difficult. In addition, the values of the three band parameters that appear in it, α, β and ω, have not been correlated to real gas data; thus, it is not immediately available for use in real gas problem solving. In this section, a simpler expression for $H_j(\kappa)$ which embodies correlated band parameters is developed.

Consider the definition of the total band absorptance $A_j(s)$ of the jth wide band of an isothermal absorbing/emitting gas (the subscript j is dropped below for convenience):

$$A(s)=\int_{\Delta\nu}[1-e^{-\kappa_\nu s}]\,d\nu. \quad (21)$$

If equation (15) is used to convert the ν integration to a κ integration, then

$$A(s)=\int_0^\infty[1-e^{-\kappa_\nu s}]H(\kappa)\,d\kappa. \quad (22)$$

This equation may be differentiated with respect to the mass path length s to give

$$\frac{dA}{ds}=\int_0^\infty\kappa e^{-\kappa s}H(\kappa)\,d\kappa. \quad (23)$$

Note that the integral on the right is in the form of a Laplace transform integral. Thus, the wide-band integration function may be obtained as an inverse Laplace transform in the same manner that the narrow-band distribution function was obtained by Domoto [7]

$$\kappa H(\kappa)=L^{-1}\left[\frac{dA(s)}{ds}\right]. \quad (24)$$

A convenient expression for $A(s)$ is needed for use in equation (24). In this study the Tien and Lowder correlation [10] is employed because it is a simple, continuous function whose derivative dA/ds is a quotient of polynomials. In addition, the Tien and Lowder expression, though derived basically from a knowledge of the mathematical behavior of $A(s)$, was also developed so as to conform closely with the Edwards correlated piece-wise expression. Thus, it can be immediately used in the solution of radiant transfer problems in the four combustion gases for which the correlated parameters α, β and ω are available. (Complete values for these parameters can be found readily, as, for example, in ref. [11].)

The Tien and Lowder [10] expression for the total band absorptance is given by

$$\bar A(\bar s)=\frac{A}{\omega}=\ln\left[\bar s f_2\left(\frac{\bar s+c}{\bar s+cf_2}\right)+1\right] \quad (25)$$

$$f_2=2.94[1-e^{-2.6\beta}]$$

where $\bar S=(\alpha/\omega)S$ and $c=2$.

Use of the latter in equation (24) produces an expression for $H(\kappa)$ that becomes negative over some ranges of κ. In order to avoid this complication, the following 'modified' c is used:

$$c = \begin{cases} 2 & \beta < 0.203 \\ \left(2 - \dfrac{1}{f_2}\right) + 2\sqrt{1 - \dfrac{1}{f_2}} & \beta \geqslant 0.203. \end{cases} \quad (26)$$

It should be noted that this 'modification' of the Tien and Lowder total band absorptance does not invalidate their original formulation. Tien and Lowder considered the mathematical properties that the total band absorptance must exhibit and obtained, from these properties, the expression shown in (25). The actual value of $c = 2$, however, was chosen by them to give a reasonable match to the Edwards piece-wise smooth expression. (The band parameters α, β and ω had already been correlated for several combustion gases for Edwards' piece-wise expression and matching this expression circumvented the time-consuming chore of re-correlating these parameters.) The modified expression used here is exactly that of Tien and Lowder for $\beta < 0.203$, and for $\beta \geqslant 0.203$ appears to match Edwards' expression at least as well as the original expression. A comparison between the modified Tien and Lowder and the Edwards expressions for A is shown in Fig. 1 for various values of β.

The expression for $H(\kappa)$ derived from the modified Tien and Lowder total band absorptance is then

$$\bar{H}(\kappa) = \frac{H}{\omega} = \frac{1}{\kappa}[e^{-a_1\kappa} + e^{-a_2\kappa} - e^{-a_3\kappa}] \quad (27)$$

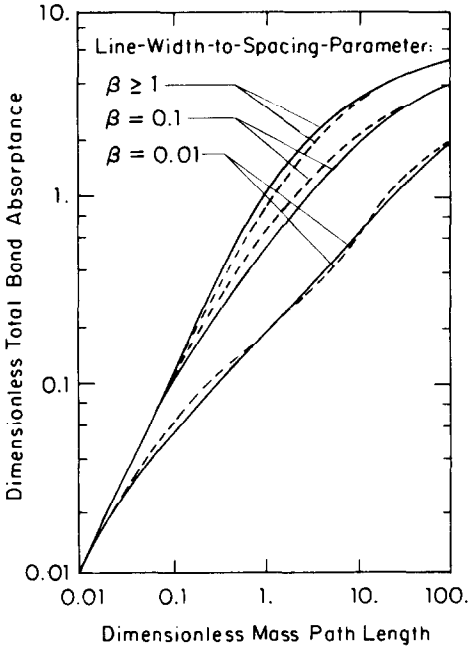

FIG. 1. Total band absorptance calculated for different β (line width to spacing parameter) from Edwards expressions ———; modified Tien and Lowder expression [equation (26)] – – – –.

$$a_1 = \frac{\omega}{2\alpha f_2}[(1 + cf_2) + \sqrt{(1 + cf_2)^2 - 4cf_2^2}] \quad (28a)$$

$$a_2 = \frac{\omega}{2\alpha f_2}[(1 + cf_2) - \sqrt{(1 + cf_2)^2 - 4cf_2^2}] \quad (28b)$$

$$a_3 = \frac{\omega}{\alpha} cf_2. \quad (28c)$$

Because equation (27) is in the form of a series of exponentials, it is particularly accessible to the numerical integration scheme known as Gauss–Laguerre quadrature [12]. In this scheme, the integral of a general function $F(x)$ over all x is approximated by

$$\int_0^\infty F(x)\, e^{-x}\, dx \approx \sum_{n=1}^{N} w_n F(x_n). \quad (29)$$

The weight factors w_n and the zeroes x_n of the N-degree Laguerre polynomial $L_N(x)$ in this equation are tabulated in many texts. (See, for example, ref. [12].)

Use of equation (29) allows total radiative quantities to be expressed as a weighted sum of gray gases. To illustrate, consider the wavenumber integration of a general radiative function of the absorption coefficient, $g(\kappa_\nu)$, that is both continuous in κ and identically zero outside of the absorption/emission band interval

$$g = \int_0^\infty g_\nu\, d\nu = \sum_{j\,\text{bands}} \int_{\Delta\nu} g(\kappa_\nu)\, d\nu$$

$$= \sum_{j\,\text{bands}} \int_0^\infty g(\kappa) H_j(\kappa)\, d\kappa$$

$$= \sum_{j\,\text{bands}} \omega_j \int_0^\infty g(\kappa)[(e^{-a_1\kappa} + e^{-a_2\kappa} - e^{-a_3\kappa})/\kappa]\, d\kappa$$

$$\approx \sum_{j\,\text{bands}} \omega_j \sum_n \frac{w_n}{x_n}\left[g\left(\frac{x_n}{a_{1_j}}\right) + g\left(\frac{x_n}{a_{2_j}}\right) - g\left(\frac{x_n}{a_{3_j}}\right)\right].$$

Thus the total function is expressible as the weighted sum of gray gases with constant absorption coefficient, $\kappa = x_n/a_{ij}$.

4. RADIANT TRANSFER BETWEEN PARALLEL PLATES WITH AN ISOTHERMAL GAS

As an illustration of the use of the integration kernel in enclosures, consider the special case of two parallel plates, separated by an absorbing/emitting gas of mass path length D and temperature T_g, in which one plate is black ($\varepsilon_1 = 1$) and the second is cold (the emissive power, $e_{b\nu 2} = 0$) and non-absorbing. This system is mathematically equivalent to one consisting of two parallel black plates at the same temperature, separated by a gas of length $2D$. An 'exact' solution (i.e. one in which all the integrals can be obtained in closed form) for the latter system can be developed as in ref.

[13]. Thus a means of evaluating both the conventional solution method (using the total band absorptance directly) and the proposed wide-band kernel substitution method is available.

For the equivalent exact system, the wall flux, q_1, may be written in terms of the total band absorptance. Then, using the Tien–Lowder expression for the total band absorptance given in equation (25), the 'exact' radiant flux supplied to each wall is

$$q_1 = \sum_j \omega_j [e_{bv_j,1} - e_{bv_j,g}] \left\{ \frac{A_j(2\bar{D})}{\omega_j} + 2\bar{D} - (2D)^2 \left[\frac{1}{a_1^2} \ln\left(1 + \frac{a_1}{2\bar{D}}\right) + \frac{1}{a_2^2} \ln\left(1 + \frac{a_2}{2D}\right) - \frac{1}{a_3^2} \ln\left(1 + \frac{a_3}{2D}\right) \right] \right\} \quad (30)$$

where

$$\bar{D} = \frac{\alpha_j}{\omega_j} D.$$

For the actual system, the wall flux is

$$q_1 = \int_0^\infty [e_{bv,1} - e_{bv,g}][1 - 4E_3^2(\kappa_v D)] \, dv \quad (31)$$

where E_3 is the third exponential integral.

Using the wide-band kernel substitution method introduced in the previous section, the total flux of surface 1 may be obtained as

$$q_1 \approx \sum_j [e_{bv_j,1} - e_{bv_j,g}] \int_0^\infty [1 - 4E_3^2(\kappa D) H_j \, d\kappa. \quad (32)$$

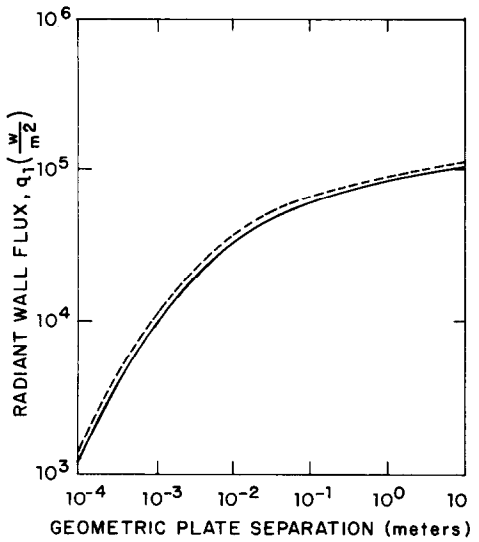

FIG. 2. Comparison of wide-band integration methods for two parallel walls, one hot (1389 K) and black and the second cold (0 K) and non-absorbing separated by CO_2 at 2778 K and 1 atm. Flux calculated for the 4.3 μm band using an equivalent exact method ———; wide-band integration kernel – – – – –.

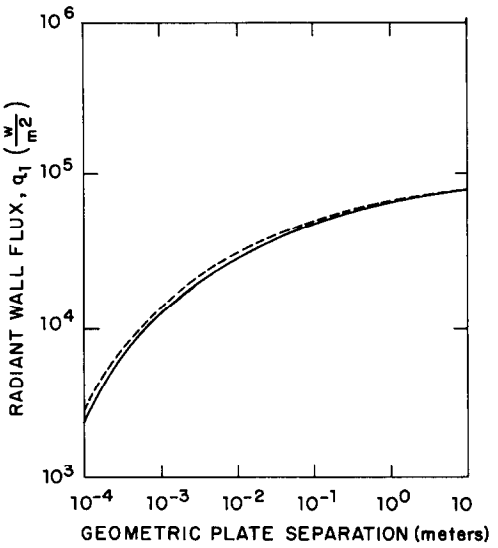

FIG. 3. Comparison of wide-band integration methods for two parallel walls, one hot (2778 K) and black and the second cold (0 K) and non-absorbing separated by CO_2 at 1389 K and 1 atm. Flux calculated for the 4.3 μm band using an equivalent exact method ———; wide-band integration kernel – – – – –.

Taking advantage of the exponential form of $H_j(\kappa)$ given in equation (27) numerical integration may be performed using Gauss–Laguerre quadrature.

Heat fluxes were calculated for two cases. In the first, hot CO_2 gas, $T_1 = 2778$ K (5000 R) is radiating to a cool black wall, $T_1 = 1389$ K (2500 R). The results are shown in Fig. 2 for geometric paths ranging from 10^{-4} m to 10 m (optical paths ranging from approximately 10^{-1} to 10^3). In the second case, a hot wall at 2778 K radiates to a 1389 K gas. The fluxes are shown in Fig. 3 for geometric paths ranging from 10^{-4} m to 10 m (optical paths from 10^{-1} to 10^4). For simplicity, fluxes from the 4.3 μm CO_2 band only were considered. In both cases, the integration kernel gives results which are within 10% of the 'exact' solution.

5. CONCLUSIONS

A wide-band integration kernel has been introduced as an extension of the narrow-band absorption coefficient distribution function. Expressions for the wide-band kernel have been developed from the exponential wide-band model and from the inverse Laplace transform of the derivative of the total band absorptance with respect to path length. The use of the latter method has been illustrated using the Tien and Lowder correlation.

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UN NOYAU D'INTEGRATION SUR LE COEFFICIENT D'ABSORPTION A LARGE BANDE

Résumé—Le concept de noyau d'intégration sur le coefficient d'absorption à large bande est introduit et développé pour l'utiliser dans les problèmes de transfert thermique par rayonnement des gaz absorbants et émetteurs. Pour chacune des bandes non transparentes d'un gaz, le noyau transforme les intégrations sur le nombre d'onde en des intégrations plus aisées sur le coefficient d'absorption. Une expression simple pour le noyau d'intégration est développée à partir de l'expression de Tien et Lowder pour l'absorptance totale de bande. L'utilisation du noyau est alors illustrée et comparée avec une solution exacte pour un exemple d'un gaz isotherme entre deux plans parallèles et infinis.

EIN INTEGRATIONS-KERN FÜR DEN BREITBANDABSORPTIONSKOEFFIZIENTEN

Zusammenfassung—Es wird das Konzept eines Integrations-Kernes für den Breitbandabsorptionskoeffizienten eingeführt und für den Gebrauch bei Problemen der Wärmeübertragung durch Strahlung in real absorbierenden/emittierenden Gasen weiterentwickelt. Für jedes der nicht-transparenten Absorptions/Emissionsbänder eines Gases, transformiert der Kern die ausführlichen Integrationen über die Wellenlänge in bequemere Integrationen über den Absorptionskoeffizienten. Aus dem Ausdruck von Tien und Lowder wurde ein einfacher Integrations-Kern für die Absorption über die gesamte Bandbreite entwickelt. Der Gebrauch des Kernes wird erläutert und mit der exakten Lösung anhand eines Beispieles mit isothermem Gas zwischen zwei unendlich großen, parallelen Platten verglichen.

ЯДРО ИНТЕГРАЛЬНОГО ПРЕОБРАЗОВАНИЯ ДЛЯ КОЭФФИЦИЕНТА ШИРОКОПОЛОСНОГО ПОГЛОЩЕНИЯ

Аннотация—Введено понятие ядра интегрального преобразования для коэффициента широкополосного поглощения, которое применимо в задачах радиационного теплопереноса в реальных поглощающих/испускающих газах. Для каждой из непрозрачных поглощающей/испускающей полос газа использование ядра позволяет перейти от интегрирования по волновому числу к удобному интегрированию. Из выражения Тьена и Лаудера для суммарного поглощения полосы получено простое ядро интегрирования. Далее приводится иллюстративный пример ядра интегрирования; полученные результаты сравниваются с точным решением для изотермического газа между двумя бесконечными параллельными пластинами.