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Technical Note

Improved band parameters for a simplified wide band cumulative absorption coefficient distribution model for H_2O and CO_2

Jing He, Richard O. Buckius *

Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, 1206 West Green Street, Urbana, IL 61801, USA

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Abstract

An accurate and computationally efficient approach to evaluate wide band parameters with polynomial series for use in a simplified wide band cumulative absorption coefficient distribution, $g(k)$, model is presented. The fitting coefficients are determined by a best fit with $g(k)$ functions generated from the latest high resolution spectroscopic database. The approach significantly improves the prediction of the $g(k)$ function over a wide range of temperatures from 500 to 2500 K, pressures from 0.01 to 1.0 atm, and all single bands of H_2O and CO_2. The root mean square error of the predicted absorption coefficient is below 25% except the single 4.3 μm band model. The approach also provides accurate calculations for the wide band absorptance, generally with differences below 7% when compared to benchmark results.

Keywords: Polynomial series; *g*-distribution; Band parameters; Wide band absorptance

1. Introduction

The cumulative k-distribution, $g(k)$, method has become increasingly important and a powerful method to model radiative heat transfer in nongray media due to the fundamental characteristics of the absorption coefficient in the solution of radiative transfer equation (RTE). The approach also outperforms the traditional spectral model in that it can be used to accurately solve radiative transport problems in highly nonhomogeneous media [1–3], in the presence of scattering particles [2,4], and in arbitrary enclosures.

Marin and Buckius develop a simplified yet accurate wide band $g(k)$ model for H_2O [5] and CO_2 [6] which explicitly expresses the absorption coefficient in terms of the cumulative distribution function. Based upon the exact expressions of the cumulative distribution function for small and large pressure limits [7], the model employs the exponential wide band model [8] together with the Malkmus model [9] plus additional physically-justified approximations. The model also introduces a fitting function to extend the pressure range to intermediate values. The invertible feature of the cumulative distribution function significantly reduces the computational expense. By adjusting band parameters using the line-by-line calculation together with the recent high-resolution spectroscopic databases, accurate and efficient radiative transport predictions are now possible.

This research presents an approach to improve the accuracy of the original model parameters for all the single bands of H_2O and CO_2. The wide band parameters are expanded in a polynomial series as a function of gas temperature, and the fitting coefficients are determined by making a best fit with $g(k)$ functions generated from the HITEMP-2000 [10] database for H_2O, and the CDSD-1000 [11] database for CO_2 over a wide range of temperatures and partial pressures. The root mean square error of the predicted absorption coefficient and wide band absorptance is presented. Significant improvement is achieved compared to the original parameter set. Calculations per-

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* Corresponding author. Tel.: +1 217 333 1079; fax: +1 217 244 6534.
E-mail address: buckius@uiuc.edu (R.O. Buckius).

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Nomenclature

a, b, c	fitting coefficients
A	wide band absorptance, cm^{-1}
A^*	nondimensional wide band absorptance
B	pressure broadening parameter (line overlap parameter)
f	distribution function
g	cumulative absorption coefficient distribution function
k	absorption coefficient, m^2/g
N	number of elements in summation
P_e	effective pressure
R	ratio, $R = s_{\max}/s_{\min}$
s	ratio between the line intensity and the line spacing, m^2/g
T	temperature, K
u	mass pathlength, g/m^2
w	weight factor for Gaussian integration
W	fitting function
Greek symbols	
κ	nondimensional absorption coefficient
α	integrated band intensity, $\text{cm}^{-1}\ \text{m}^2/\text{g}$
γ	line overlap parameter for dilute gas
ω	bandwidth parameter, cm^{-1}
η	wavenumber, cm^{-1}
$\Delta\eta$	wavenumber interval, cm^{-1}
Subscripts	
0	band center or band head, reference band parameters
i, j, k	summation parameter
min	minimum value
max	maximum value
t	transition
low	lower limit
up	upper limit
WB	wide band $g(k)$ model
LBL	line-by-line calculation

formed along a homogeneous and isothermal gas column show that the $g(k)$ model employing the new parameters provides much more accurate results in band absorptance than the exponential wide band model [8].

2. Wide band $g(k)$ formulation

2.1. Single and overlapped transition band formulation

Wide band spectral intervals can be classified into three distinct categories – single, overlapped and multiple [7]. For single and overlapped bands, Marin and Buckius [7] develop limiting forms of the wide band absorption coefficient distribution for small and large pressures. Extending this approach, a continuous stepwise formulation [5,6] for the cumulative distribution function is proposed as

$$g(\kappa) = \begin{cases} 0, \\ \quad \text{for } \kappa \leqslant e^{2e^{-B/4} - W(B,R)\ln(R)} \\ W(B,R) + \frac{1}{\ln(R)}\left[\ln(\kappa) - 2e^{-B/4}\right], \\ \quad \text{for } e^{2e^{-B/4} - W(B,R)\ln(R)} < \kappa \leqslant R \\ 1 + W(B,R) - \frac{2e^{-B/4}}{\ln(R)}\sqrt{\frac{R}{\kappa}}, \\ \quad \text{for } R < \kappa \leqslant \kappa_{\max} \\ 1, \\ \quad \text{for } \kappa_{\max} < \kappa \end{cases} \tag{1}$$

The nondimensional absorption coefficient, κ, defined as

$$\kappa = \frac{k}{s_{\min}(1 - e^{-B})} \tag{2}$$

is obtained directly through analytical inversion of Eq. (1) as

$$\kappa(g) = \begin{cases} e^{[g - W(B,R)]\ln(R) + 2e^{-B/4}}, \\ \quad \text{for } 0 \leqslant g \leqslant 1 + W(B,R) - \frac{2e^{-B/4}}{\ln(R)} \\ R\left[[1 + W(B,R) - g]\frac{\ln(R)}{2e^{-B/4}}\right]^{-2}, \\ \quad \text{for } 1 + W(B,R) - \frac{2e^{-B/4}}{\ln(R)} < g \leqslant 1 \end{cases} \tag{3}$$

The pressure broadening parameter, B, and the ratio between the maximum and the minimum line-intensity to spacing ratio in a wide band interval, R, are the two required model parameters. Both are related to the same wide band parameters defined in Edwards' exponential wide band model [8] through

$$B = \gamma P_e \tag{4}$$

$$R = \frac{s_{\max}}{s_{\min}} = \frac{\frac{\alpha}{\omega}}{\frac{\alpha}{\omega}\exp\left(-\frac{\eta_{\text{up}} - \eta_{\text{low}}}{\omega}\right)} = \exp\left(\frac{\eta_{\text{up}} - \eta_{\text{low}}}{\omega}\right) = \exp\left(\frac{\Delta\eta}{\omega}\right) \tag{5}$$

η_{up} and η_{low} are the upper and lower limits for a wide band interval $\Delta\eta$, respectively, which are specified in this $g(k)$ model and maintained constant as prescribed. Thus, different bands remain distinct in all cases. The fitting function $W(B,R)$ is introduced to account for intermediate values of B, expressed as

$$W(B,R)=\frac{2\mathrm{e}^{-B/4}}{\ln(R)}\sqrt{\frac{(1-\mathrm{e}^{-B})[\cosh(2\pi B)-1]}{\sinh(2\pi B)}} \tag{6}$$

The maximum nondimensional absorption coefficient required in the limits of Eq. (1), $\kappa_{\max}$, is derived from the maximum value given by the Elsasser narrow band formulation for the spectral absorption coefficient combined with Eqs. (2) and (5)

$$\kappa_{\max}=\frac{k_{\max}}{s_{\min}(1-\mathrm{e}^{-B})}=\frac{s_{\max}\frac{\sinh(2\pi B)}{\cosh(2\pi B)-1}}{s_{\min}(1-\mathrm{e}^{-B})}=\frac{R}{1-\mathrm{e}^{-B}}\cdot\frac{\sinh(2\pi B)}{\cosh(2\pi B)-1} \tag{7}$$

2.2. Multiple band formulation – 4.3 μm band of carbon dioxide

As noted in Refs. [6,7], the 4.3 μm band of CO_2 is more accurately represented as a multiple, separated band characterized by the presence of distinct and independent rotational–vibrational transitions. A multiple band formulation is employed in the form of

$$g(k)=\sum_{i=1}^{N_t}\frac{\Delta\eta_i}{\Delta\eta}g_i(k) \tag{8}$$

where N_t is the number of dominant transitions within the spectral interval considered $\Delta\eta$. The transition i is dominant on the spectral interval $\Delta\eta_i$ and is represented by the cumulative distribution function $g_i(k)$. Three vibrational transitions dominate in the 4.3 μm region, characterized by a change in the quantum numbers of $(1,1,0)$, $(2,-1,0)$ and $(0,0,1)$. In this study, the individual spectral interval $\Delta\eta_i$ is taken to be constant for all gas conditions (pressure, temperature and concentration). This procedure is justifiable considering that different transitions are dominant on separate spectral regions, as shown by Taine and coworkers [12]. Optimal limits for the three spectral intervals are found to be $(1950,2125)$, $(2125,2220)$ and $(2220,2400)\,\mathrm{cm}^{-1}$, corresponding to the transitions $(1,1,0)$, $(2,-1,0)$ and $(0,0,1)$ respectively. The multiple cumulative distribution function for the 4.3 μm band is then expressed as

$$g(k)=\frac{175}{450}g_1(k)+\frac{95}{450}g_2(k)+\frac{180}{450}g_3(k) \tag{9}$$

The individual cumulative distribution function $g_i(k)$ is described by Eq. (1). Consequently, three sets of band parameters are now required in Eq. (9).

For the 4.3 μm band, both the single band model in Section 2.1 and the multiple band model in this section are presented.

3. Band parameters

Marin and Buckius [7] indicate that the appropriate band parameters are dependent on the particular benchmark results employed, and a different database would yield a slightly different parameter set. The previous parameters presented in Refs. [5,6] were based upon the HITEMP line-by-line database [10] for temperatures up to 1000 K, and the EM2C narrow-band database [13] above 1000 K. In this study, HITEMP is extended to use for temperatures up to 2500 K for H_2O, and the recent and more accurate CDSD-1000 database [11] is employed for CO_2. Such choices have been justified by the latest research of Wang and Modest [14].

The traditional approach to evaluate wide band parameters by directly computing the function $\Psi(T)$ appearing in α and the function $\Phi(T)$ appearing in γ significantly increases the computing time of the total radiative properties. To address the computational difficulty, Lallemant and Weber [15] propose very simple yet accurate polynomial fits for these functions, and the fitting coefficients are determined by minimizing the difference comparing with the exact equations. This study adopts a similar procedure, with the benchmark now being $g(k)$ functions generated from the line-by-line calculation using the latest version of high-resolution databases. The three parameters for all bands follow the same functional form, varying solely with temperature as

$$\alpha=\alpha_0\cdot\left(\sum_{i=0}^{N}a_iT^i\right) \tag{10a}$$

$$\gamma=\gamma_0\cdot\left(\sum_{j=0}^{N}b_jT^j\right) \tag{10b}$$

$$\omega=\omega_0\cdot\left(\sum_{k=0}^{N}c_kT^k\right) \tag{10c}$$

(α_0, γ_0, ω_0) are constant band parameters. The fitting coefficients (a_i,b_j,c_k) for a particular wide band interval are optimized for temperatures in the range 500–2500 K (with temperature limitation of 500–2000 K for the pure rotational band; 1000–2500 K for the 1.38 μm band of H_2O; 500–1500 K for the 15.0, 10.4, and 9.4 μm bands of CO_2; for other temperatures, the contributions from these relatively weak bands are negligible), and for partial pressures in the range 0.01–1.0 atm. The total pressure is fixed at 1.0 atm throughout this study.

Table 1 presents the new constant band parameters and the fitting coefficients for all the vibrational–rotational bands of H_2O and CO_2. A fourth-order polynomial is found to provide the best compromise between the accuracy and the number of terms in power series over the entire temperature region. Note that the parameters for the 4.3 μm band of CO_2 in Table 1 are to be used in the single band formulation of Eq. (1). Those for use in the multiple band formulation of Eq. (9) are listed in Table 2. A maximum power of six is required for parameters used in each individual cumulative distribution function, indicating the complexity of this particular spectral interval.

Table 1
Constant parameters and fitting coefficients for use in polynomial series (Eqs. (10a)–(10c)) for all the single band models of H_2O and CO_2 (Eq. (1))

Band (μm)	H_2O					CO_2					
	Rot.	6.3	2.7	1.87	1.38	15.0	10.4	9.4	4.3	2.7	2.0
η_{low}	10	1000	2600	4400	6000	450	850	1000	1950	3300	4700
η_{up}	1000	2600	4400	6000	8000	850	1000	1125	2400	3800	5250
α_0	420	39.6	25.8	2.80	2.17	12.3	0.32	0.58	117	4.30	1.20
γ_0	0.114	0.094	0.080	0.085	0.118	1.50	0.404	0.025	0.247	0.233	0.555
ω_0	69.3	72.8	83.0	70.6	78.0	30.0	510	100	3.43	22.1	65.0
α (*Eq.* (10a))											
a_0	0.46059	0.85304	0.96511	0.94655	0.86195	0.44648	0.05933	0.10327	0.90755	0.97517	0.10187
$a_1(\times 10^4)$	−2.33682	1.84771	0.94133	−0.15269	5.64164	8.22982	−4.66766	−5.49818	8.12314	−2.02215	−1.89288
$a_2(\times 10^7)$	1.82116	−1.76254	−2.60162	−0.29697	−8.24969	−2.66739	9.74177	9.59589	−5.91575	2.13581	2.92922
$a_3(\times 10^{10})$	−0.77097	0.96722	1.59307	1.83124	4.43978	0	−2.29337	−2.87222	0.59237	2.12801	−1.22006
$a_4(\times 10^{14})$	1.42594	−1.88899	−2.87523	−4.72511	−7.64231	0	0	0	1.57190	−7.89527	1.54239
γ (*Eq.* (10b))											
b_0	0.33279	0.26627	0.05557	−0.26799	−0.97077	−0.49434	−0.43753	6.66155	2.63189	−2.39061	−1.66149
$b_1(\times 10^3)$	0.18623	0.69833	1.02994	1.97772	3.89992	2.60011	2.54811	−5.26860	−8.21982	9.94018	6.95882
$b_2(\times 10^6)$	−0.25732	−0.80705	−0.97601	−1.69479	−3.89148	−4.17849	−4.01060	3.77203	9.86618	−7.94209	−8.84911
$b_3(\times 10^9)$	0.17860	0.51037	0.57023	0.79261	1.80726	3.09092	2.91726	2.63636	−2.15478	2.98433	4.62184
$b_4(\times 10^{13})$	−0.30817	−0.92004	−0.97755	−1.14736	−2.69634	−7.95843	−7.52527	0	0	−3.59149	−7.73717
ω (*Eq.* (10c))											
c_0	0.63762	1.38608	1.79076	2.28397	4.31320	1.11221	0.88175	0.70054	3.22138	4.24069	−1.78468
$c_1(\times 10^3)$	1.81588	0.35094	0.03373	−2.22995	−6.85559	−1.24593	−3.49494	−2.81561	7.23678	−8.73154	9.50487
$c_2(\times 10^6)$	−1.33278	2.71457	1.64334	4.45173	8.59305	4.15601	5.98883	5.93524	−0.64268	9.78168	−5.70016
$c_3(\times 10^9)$	1.25613	−1.45599	−0.56026	−1.64418	−3.34007	−2.79807	−4.05890	−4.15631	0.17117	−1.87267	1.36068
$c_4(\times 10^{13})$	−3.30484	2.21603	0.51098	1.87399	4.41954	6.42984	9.84969	9.87497	0	0	−1.04515

Table 2
Fitting coefficients for use in polynomial series (Eqs. (10a)–(10c)) for the 4.3 μm multiple band model (Eq. (9))

	Transition $(1,1,0)$ $g_1(k)$	Transition $(2,-1,0)$ $g_2(k)$	Transition $(0,0,1)$ $g_3(k)$
α (*Eq.* (10a))			
a_0	1.87351×10^{-1}	-1.95468×10^{-1}	1.13575×10^{2}
a_1	-1.39419×10^{-3}	-2.84524×10^{-3}	1.98183×10^{-1}
a_2	3.87600×10^{-6}	2.16785×10^{-5}	-5.79062×10^{-4}
a_3	-4.69181×10^{-9}	-5.08587×10^{-8}	7.57670×10^{-7}
a_4	2.48374×10^{-12}	5.02143×10^{-11}	-4.53624×10^{-10}
a_5	-4.21066×10^{-16}	-1.90034×10^{-14}	1.24151×10^{-13}
a_6	0	2.47191×10^{-18}	-1.27336×10^{-17}
γ (*Eq.* (10b))			
b_0	-2.47461×10^{0}	7.10066×10^{0}	1.69140×10^{0}
b_1	7.81651×10^{-3}	-3.42121×10^{-2}	-8.34569×10^{-3}
b_2	-6.76741×10^{-6}	5.98882×10^{-5}	1.72898×10^{-5}
b_3	2.39896×10^{-9}	-4.74648×10^{-8}	-1.75331×10^{-8}
b_4	0	1.84373×10^{-11}	9.24873×10^{-12}
b_5	0	-3.28547×10^{-15}	-2.39022×10^{-15}
b_6	0	1.94271×10^{-19}	2.39480×10^{-19}
ω (*Eq.* (10c))			
c_0	1.89670×10^{3}	5.98161×10^{2}	-2.32193×10^{1}
c_1	-8.47025×10^{0}	-2.29787×10^{0}	2.76913×10^{-1}
c_2	1.54152×10^{-2}	3.66241×10^{-3}	-7.33145×10^{-4}
c_3	-1.43182×10^{-5}	-3.03240×10^{-6}	1.08411×10^{-6}
c_4	7.16906×10^{-9}	1.38675×10^{-9}	-7.50364×10^{-10}
c_5	-1.84251×10^{-12}	-3.31090×10^{-13}	2.41480×10^{-13}
c_6	1.90742×10^{-16}	3.22349×10^{-17}	-2.94029×10^{-17}

The upper limit for the 4.3 μm region is 2400 cm^{-1}, and the lower limit is 1950 cm^{-1}, within which (1950, 2125), (2125, 2220), (2220, 2400) are the spectral intervals corresponding to the three transitions $(1,1,0)$, $(2,-1,0)$, and $(0,0,1)$, respectively. Use $\alpha_0 = \gamma_0 = \omega_0 = 1$ in Eqs. (10a)–(10c) for individual function $g_1(k)$, $g_2(k)$, $g_3(k)$.

Table 3 shows the averaged root mean square error produced by the $g(k)$ model. For a particular band at a given temperature and partial pressure, the values of 32-point Gaussian quadrature abscissas between 0 and 1 are preselected for the cumulative distribution function. The root mean square error is computed for absorption coefficients corresponding to $g(k) > 0.2$ [5,6] by

$$\text{RMS}_k = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{k_{\text{WB}} - k_{\text{LBL}}}{k_{\text{LBL}}}\right)^2} * 100\% \tag{11}$$

where $N = 23$ according to the above definition. k_{WB} is the absorption coefficient predicted by the model via Eq. (3), and k_{LBL} refers to the benchmark results obtained through the line-by-line calculation. The RMS_k errors for the designated range of temperatures and partial pressures are then averaged to get the values presented in Table 3. It is noted that all the band models produce an error below 25% except the single 4.3 μm band model. As aforementioned, the single band model is less accurate than the multiple band model with the value of RMS_k increased by a factor of 2. However, Eq. (9) cannot be inverted analytically, thus losing an important computational feature of the single band formulation (Eq. (1)). The Brent's algorithm on root finding [16] is used in this study to solve for the absorption coefficient numerically. In addition, the relatively large errors for the pure rotational band result from the assumption of a fully symmetric wideband and decaying to zero in both wings as used in the exponential wide band model.

Fig. 1 illustrates typical cumulative distribution functions for the 2.7 μm H_2O band, the 2.7 μm CO_2 band, and the 4.3 μm CO_2 band, obtained from the line-by-line calculation and the wide band $g(k)$ model using the parameters in Table 1 for the single band formulation and the parameters in Table 2 for the multiple band formulation. The model is in good agreement with the benchmark results for large domains of the cumulative distribution function. For the single band model, differences occur for small values of the absorption coefficient that are of less importance in many engineering applications. Due to the interaction between different rotational–vibrational transitions, the cumulative distribution function for the 4.3 μm region has a much more complicated dependence on the absorption coefficient than other bands, which are accurately described by the multiple band formulation together with the suggested band parameters in Table 2. The multiple band model is able to yield accurate prediction for the absorption coefficient in the entire distribution range, $0 < g(k) < 1$. Its superiority over the single band model is clearly exhibited in Fig. 1a and d.

4. Wide band absorptance comparisons

For any spectral quantity that depends solely on the gaseous absorption coefficient, the integration over the wavenumber can be replaced by the integration over the absorption coefficient, and alternatively, over the cumulative distribution function. This concept can be applied to a wide band spectral region in which the line spectrum is of arbitrary complexity, provided that the Planck function may be assumed to be constant [1]. The wide band absorptance within a considered interval $\Delta\eta$ at the mass path length u is defined as

Table 3
Root mean square error of the predicted absorption coefficients (RMS_k, %) for all H_2O and CO_2 bands corresponding to $g(k) > 0.2$, in the partial pressure range 0.01–1.0 atm, and the temperature range 500–2500 K unless otherwise specified[a]

Band [μm]	H_2O					CO_2					
	Rotational	6.3	2.7	1.87	1.38	15.0	10.4	9.4	4.3	2.7	2.0
RMS_k	24.9	16.0	19.5	19.4	23.8	21.4	19.2	15.4	$47.6^{\text{Single}}/24.5^{\text{Multiple}}$	22.9	13.3

[a] 500–2000 K for the pure rotational band; 1000–2500 K for the 1.38 μm band; 500–1500 K for the 15.0, 10.4 and 9.4 μm bands.

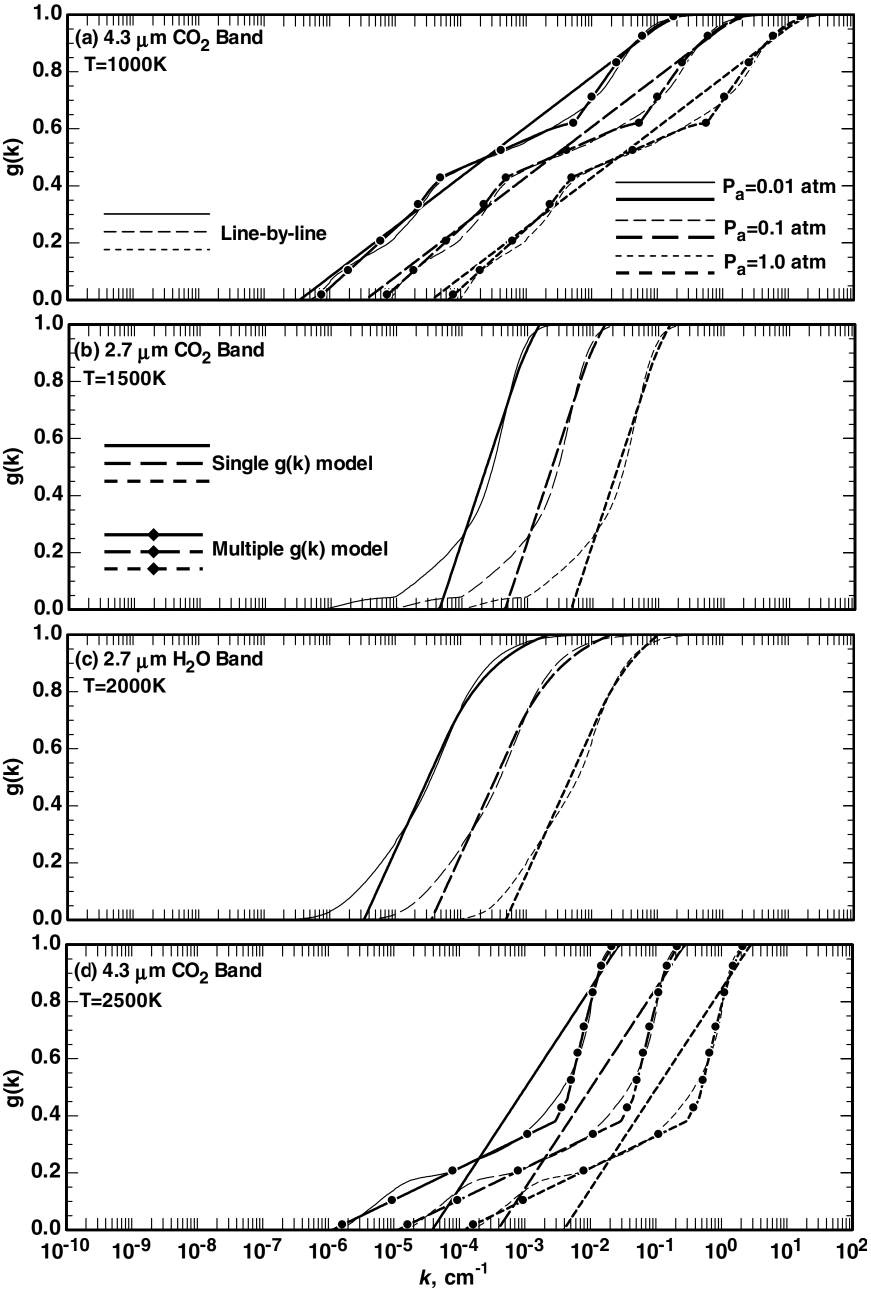

Fig. 1. Cumulative k-distribution function, for (a) the 4.3 μm CO_2 band at 1000 K, (b) the 2.7 μm CO_2 band at 1500 K, (c) the 2.7 μm H_2O band at 2000 K, (d) the 4.3 μm CO_2 band at 2500 K, and partial pressures 0.01, 0.1, 1.0 atm. The total pressure is fixed at 1.0 atm. The plain lines represent the line-by-line calculations [10,11]; the bold lines represent the single band model described by Eq. (1); the marked lines in (a) and (d) represent the multiple band model described by Eq. (9) for the 4.3 μm band.

$$A = \int_{\Delta\eta} (1 - \mathrm{e}^{-k_\eta u})\mathrm{d}\eta \tag{12}$$

Nondimensionalized with the bandwidth parameter ω, the integral can be written as

$$\begin{aligned} A^* &= \frac{A}{\omega} = \frac{\Delta\eta}{\omega}\int_0^\infty (1 - \mathrm{e}^{-ku}) f(k)\mathrm{d}k \\ &= \frac{\Delta\eta}{\omega}\int_0^1 (1 - \mathrm{e}^{-k(g)u})\mathrm{d}g \end{aligned} \tag{13}$$

A 32-point Gaussian quadrature scheme is employed for numerical integration of Eq. (13) through

$$A^* = \frac{\Delta\eta}{\omega}\sum_{i=1}^{N_q} (1 - \mathrm{e}^{-k_i(g_i)u}) w_i \tag{14}$$

where the quadrature number $N_q = 32$, and w_i are the weight factors. The values of g_i are determined by the abscissas for Gaussian integration, and k_i are the corresponding absorption coefficient.

Table 4
Root mean square error of the wide band absorptance (RMS_A, %) for all H_2O and CO_2 bands, for pressure path lengths between 10^{-4} and 10^1 atm m, and temperatures between 500 and 2500 K (500–2000 K for the pure rotational band; 1000–2500 K for the 1.38 μm band; 500–1500 K for the 15.0, 10.4 and 9.4 μm bands, same as specified in Table 3)

Band (μm)	H_2O					CO_2					
	Rotational	6.3	2.7	1.87	1.38	15.0	10.4	9.4	4.3	2.7	2.0
$g(k)$	6.6	3.6	4.4	2.9	5.7	7.5	4.8	2.5	$16.1^{\text{Single}}/3.2^{\text{Multiple}}$	5.3	2.9
exp	390.3	21.2	18.6	18.5	31.9	40.4	14.3	17.7	11.5	24.2	42.3

$g(k)$ and exp denote predictions based upon the cumulative distribution function and the exponential wide band model, respectively.

Table 4 shows the root mean square error in the calculation of the wide band absorptance (RMS_A) for a homogeneous and isothermal gas column, for pressure pathlengths between 10^{-4} and 10^1 atm m. The temperature range for individual bands is the same as specified for developing the respective band parameters. The wide band $g(k)$ model using the new parameters and the exponential wide band model [8] (data for the pure rotational band of H_2O are taken from Modak [17]) are denoted as $g(k)$ and exp, respectively. The exact integration of Eq. (12) by the line-by-line calculation (with a spectral resolution of 0.01 cm^{-1}) in the spectral limits indicated in Table 1 for each band is considered as the benchmark result. The $g(k)$ model with the new parameters provides an accurate prediction of the wide band absorptance. Comparing to the $g(k)$ model predictions in [5,6], the RMS_A error is typically reduced by a factor of 2 and to a smaller value for the relatively weak bands –1.38 μm band and 15.0 μm band. The RMS_A error is typically reduced by a factor of 3 for all bands as compared to the exponential wide band model prediction. The root mean square errors using $g(k)$ are less than 7.5%, and decrease below 5.3% for the stronger bands (6.3 μm and 2.7 μm H_2O bands; 4.3 μm and 2.7 μm CO_2 bands). Note that the multiple band formulation for the 4.3 μm band significantly improves the prediction of band absorptance comparing with the single band formulation.

In this work, the general expression of band absorptance is used for the pure rotational band in the exponential wide band model which accounts for the asymmetric feature within this particular spectral interval [18]. Significant errors occur for the small optical paths investigated (as low as 10^{-4} atm m), which results in the large RMS_A value presented in Table 4. In the more realistic combustion conditions, typically from 0.01 to 10 atm m, the error of the exponential wide band model for the pure rotational band decrease to less than 75% for temperatures in the range 500–2000 K, and to 27% for temperatures below 1000 K. In addition, the differences in the prediction of wide band absorptance between the wide band $g(k)$ model and the exponential wide band model result from the treatment of the band limits. The $g(k)$ model specifies the band spectral limits, and different bands remain distinct in all conditions. This assumption permits the determination of the effective absorption coefficient within the spectral interval considered. While in the exponential wide band model, the bands have variable intervals and eventually overlap for large values of optical thickness.

5. Conclusions

In this study, the original band parameters [5,6] for use in a simplified wide band $g(k)$ model are improved by using the latest high-resolution databases for H_2O [10] and CO_2 [11]. Very accurate and computationally efficient polynomial series are evaluated for the three wide band parameters as a function of gas temperature. This work preserves the variation of band parameters with respect to pressure as described in the exponential wide band model [8]. The simplified model together with the new parameters accurately predict the cumulative distribution function for all the H_2O and CO_2 bands, for temperatures in the range 500–2500 K, and partial pressures in the range 0.01–1.0 atm with the total pressure fixed at 1.0 atm. The root mean square error in the predicted absorption coefficient is less than 25%, except for the 4.3 μm band, which is better represented by the proposed multiple band model.

As an application, the $g(k)$ model is employed to compute the wide band absorptance for a broad range of temperatures and pressure pathlengths, and compared with the line-by-line calculation and the exponential wide band model. The comparison shows that the model applying the new parameters yields very accurate results in band absorptance. Differences from the benchmark results are typically less than 7.5%. For those important bands in thermal transport calculations (e.g., the 6.3 μm and 2.7 μm bands of H_2O; the 4.3 μm and 2.7 μm bands of CO_2), the errors are below 5.3%. Large deviation at small optical paths as mentioned in Refs. [5,6] does not arise by employing the new parameters.

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