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A simplified wide band model of the cumulative distribution function for carbon dioxide

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Abstract

An efficient and accurate wide band absorption coefficient cumulative distribution function is used to model the 2.0, 2.7, 4.3, 9.4, 10.4 and 15.0 μm bands of carbon dioxide. Band parameters for these bands are determined, and a study of the accuracy of the formulation is performed over a wide range of pressures and temperatures. The model accurately describes the absorption coefficient distributions compared to existing line-by-line and narrow band results. The simplified formulation of the absorption coefficient provides accurate values for the wide band absorption, generally with differences below 10% when compared to benchmark results.

Nomenclature

A	wide band absorption [$\mathrm{cm^{-1}}$]
A^*	nondimensional wide band absorption
b	line halfwidth [$\mathrm{cm^{-1}}$]
B	pressure broadening parameter, $B = b/d$
d	line spacing [$\mathrm{cm^{-1}}$]
g	cumulative distribution function
k	absorption coefficient [$\mathrm{m^2\,g^{-1}}$]
L	layer thickness [m]
N	number of elements in summation
P	pressure [atm]
R	ratio, $R = s_{\max}/s_{\min}$
s	line intensity divided by line spacing [$\mathrm{m^2\,g^{-1}}$]
$s_{\min}$	minimum line intensity [$\mathrm{m^2\,g^{-1}}$]
$s_{\max}$	maximum line intensity [$\mathrm{m^2\,g^{-1}}$]
S	line intensity [$\mathrm{cm^{-1}\,(g^{-1}\,m^{-2})}$]
T	temperature [K]
u	mass pathlength [$\mathrm{g\,m^{-2}}$]
w	weight factor for Gaussian integration
W	function.

Greek symbols

α	integrated band intensity [$\mathrm{cm^{-1}\,(g^{-1}\,m^{-2})}$]
β	band parameter
δ	difference
$\Delta\nu$	wavenumber interval [$\mathrm{cm^{-1}}$]
κ	nondimensional absorption coefficient
ν	wavenumber [$\mathrm{cm^{-1}}$]
ρ	density [$\mathrm{g\,m^{-3}}$]
ω	bandwidth parameter [$\mathrm{cm^{-1}}$].

Subscripts

0	band center or band head, reference band parameters
1, 2	band indices
A	wide band absorption
c	complete model
e	exact, effective
edw	Edwards model
i	summation parameter
k	absorption coefficient
l	lower
lbl	line-by-line
m	model
max	maximum
min	minimum
nb	narrow band
q	quadrature

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1. Introduction

The solution of the radiative transfer equation for transport with participating gases requires detailed information about the gas absorption coefficient. The gas absorption coefficient varies dramatically within the infrared spectral interval, which makes the spectral integration of the transport equation computationally expensive. Different methods have been developed to evaluate and incorporate the absorption coefficient spectral variation. The only exact method to calculate the absorption coefficient is the line-by-line method. This approach estimates the magnitude of the spectral absorption coefficient directly from the participating rotational–vibrational electronic transitions. Figure 1 presents the spectral variation of pure carbon dioxide absorption coefficient over a wide infrared region, predicted from the line-by-line method [1, 2], for a pressure of 1 atm. The HITRAN database is used in Fig. 1(a) at a temperature of 500 K, while Figs 1(b) and (c) use the HITEMP database at temperatures of 750 and 1000 K, respectively. The absorption coefficient presented in Fig. 1 is averaged over spectral intervals of 5 cm^{-1}. It is observed that there are wide spectral intervals over which the absorption coefficient is very small or equal to zero, and there are also spectral intervals where the absorption coefficient is very large and highly nonuniform. It is noted that the number of lines used to calculate the cases in Figs 1(b) and (c) is in excess of one million, requiring a significant computational effort.

With the line-by-line database restricted to ambient temperature (HITRAN), and more recently to temperatures of up to 1000 K (HITEMP), a significant effort is directed towards the generation of hot lines, in order to develop high temperature line-by-line data. Taine [3] uses the low temperature database to generate hot bands, reporting results up to 3000 K. Wattson and Rothman [4, 5] use the Direct Diagonalization technique to generate hot band parameters for carbon dioxide. Using the HITRAN database, Scutaru et al. [6, 7] generate hot lines using a technique involving the diagonalization of the Fermi matrix. An approximate database for temperatures up to 3000 K is thus developed which is suitable for resolutions of a few inverse centimeter spectral intervals. The results obtained with this database are compared to experimental results up to 2850 K for the 4.3 μm band, 1500 K for the 2.7 μm band and 800 K for the 15.0, 10.9 and 9.4 μm bands.

Due to a very significant computational effort, most of the engineering heat transfer applications replace the line-by-line method with approximate methods, which evaluate the gas absorption characteristics over different spectral intervals as opposed to exact spectral locations. The magnitude of the spectral interval determines both the computational effort and the accuracy of the method employed. Soufiani and Taine [8, 9] develop band parameters for spectral intervals of 25 cm^{-1}, based upon the detailed spectral information of Scutaru et al. [7]. The band parameters presented for a wide range of pressures and for temperatures up to 2900 K are used in connection to the Malkmus [10] statistical narrow band model. The narrow band database can be used to calculate the band transmissivity and absorptivity, using the expression developed by Malkmus for the transmissivity. Alternatively, the database can be used to generate the absorption coefficient distribution function, used in connection to the *k*-distribution method. This approach replaces the spectral integration of the radiative transfer equation with an integration over the cumulative distribution function, leading to a significant reduction in computational effort. Additionally, the *k*-distribution method can be extended to nonhomogeneous media, where it is termed the correlated-*k* method. This work considers carbon dioxide based upon line-by-line calculations for temperatures up to 1000 K and compares the results with the narrow band database of Soufiani and Taine for a wide range of temperatures and pressures.

Although accurate and less computationally expensive when compared to the line-by-line method, the narrow band models require a significant computational effort when calculations over the entire infrared spectral interval are sought. A more economic approach involves modeling entire rotational–vibrational bands or wide bands involving hundreds of inverse centimeters. The most popular wide band model, developed by Edwards and co-workers [11–15], assumes an exponential variation of the average intensity-to-spacing ratio from the band center towards the band wings. Edwards calculates the band absorptivity, using simple yet accurate expressions, and develops band parameters for the most important bands of the water vapor, carbon dioxide and several other gases. Alternatively, the wide band formulation can be used together with the absorption coefficient distribution function method. Goody et al. [16] and Marin and Buckius [17] apply the correlated-*k* method by deriving *k*-distributions directly from line-by-line calculations, for different spectral intervals. Reference [17] shows that the correlated-*k* method associated to wide spectral intervals constitutes an accurate and efficient approach to highly nonhomogeneous media.

The absorption coefficient distribution functions can also be derived from the wide band model. Wang and Shi [18] develop an absorption coefficient distribution function for the Malkmus narrow band model applied to the exponential wide band model. Marin and Buckius [19] compare the wide band cumulative distribution functions resulted from different models and develop approxi-

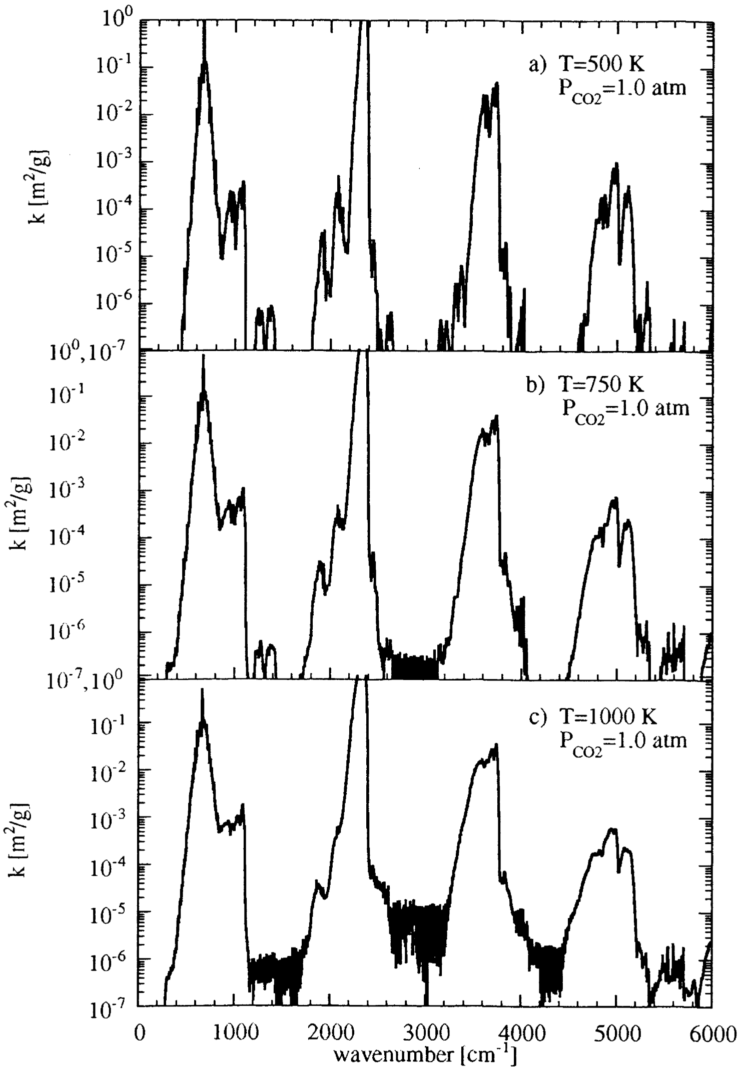

Fig. 1. Absorption coefficient variation for pure carbon dioxide with a pressure of 1 atm over the infrared spectrum, with a spectral resolution equal to 5 cm^{-1}. (a) $T = 500$ K, (b) $T = 750$ K and (c) $T = 1000$ K.

mate expressions for the absorption coefficient cumulative distribution function of the Malkmus model used with the exponential band model. The absorption coefficient distribution method is also applied to scattering media. Using an inverse Laplace transform approach, Lee et al. [20] and Parthasarathy et al. [21] calculate a reordered distribution of the absorption coefficient associated with the exponential wide band formulation. Marin and Buckius [22] develop simple, limiting expressions for the wide band absorption coefficient cumulative distribution function. It is shown that the wide band spectral intervals can be divided into three categories, depending on the transitions within the various rotational–vibrational bands. Finally, ref. [23] develops a continuous formulation for the wide band cumulative distribution function and applies it for the dominant water vapor bands, with good agreement between the model and benchmark calculations. This formulation yields an expression of the absorption coefficient in terms of the cumulative distribution function, decreasing the computational burden by around one order of magnitude when compared to alternate implicit formulations [17]. The current effort develops wide band cumulative distribution function parameters for the dominant bands of carbon dioxide, analyzing both the cumulative distribution function and the wide band absorption.

2. Wide band *g*-distribution formulation

The radiative transfer equation over a line of sight can be easily solved for a spectral location corresponding to a particular value of the absorption coefficient. The integration of the radiative transfer equation over a desired spectral interval is computationally expensive due to the highly nonuniform variation of the spectral absorption coefficient as shown in Fig. 1. Alternatively, the integration can be performed over the absorption coefficient distribution function which is a relatively smooth function that is suitable for accurate numerical integration. Thus, the evaluation of the absorption coefficient at specific spectral locations is replaced with the evaluation of the absorption coefficient for a limited number of values of the distribution function. This work is focused on the development of simple expressions for the absorption coefficient cumulative distribution function for the rotational–vibrational bands of carbon dioxide. Wide band spectral intervals can be classified into three distinct categories [22]. Wide spectral intervals dominated by one single rotational–vibrational transition and intervals with several overlapping and interacting transitions can be modeled with the same type of equations. The third category is represented by multiple bands which are dominant on different subintervals of the spectral interval considered. A modified distribution function formulation is developed for this particular case [22].

2.1. Single and overlapped transition band formulation

For single and overlapped bands, ref. [22] develops limiting forms of the wide band absorption coefficient distribution function for small and large pressures. Extending this approach, ref. [23] develops a continuous formulation for the absorption coefficient cumulative distribution function as

$$g_{\mathrm{wb}}(\kappa) = \begin{cases} 0 \\ \quad \text{for } \kappa \leqslant \mathrm{e}^{2\mathrm{e}^{-B/4} - W(B,R)\ln(R)} \\ W(B,R) + \dfrac{1}{\ln(R)}[\ln(\kappa) - 2\,\mathrm{e}^{-B/4}] \\ \quad \text{for } \mathrm{e}^{2\mathrm{e}^{-B/4} - W(B,R)\ln(R)} < \kappa \leqslant R \\ 1 + W(B,R) - \dfrac{2\,\mathrm{e}^{-B/4}}{\ln(R)}\sqrt{\dfrac{R}{\kappa}} \\ \quad \text{for } R < \kappa \leqslant \kappa_{\max} \\ 1.0 \\ \quad \text{for } \kappa_{\max} < \kappa \end{cases} \qquad \text{(1a–d)}$$

where $g_{\mathrm{wb}}(\kappa)$ is the cumulative distribution function, and κ is the nondimensional absorption coefficient defined as

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

B is the pressure broadening parameter, defined as a ratio between the absorption line halfwidth b and the average line spacing d, and $s_{\min}$ is the minimum line intensity-to-spacing ratio within the band ($s = S/d$), defined as $s_{\min} = \alpha/(\omega R)$. The band parameter α is termed the band intensity parameter, ω is the bandwidth parameter, and the ratio $R = s_{\max}/s_{\min} = \exp(\Delta v/\omega)$, where Δv is the band spectral interval. The function $W(B, R)$ is defined as

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

and is used to bridge the limiting expressions for general values of the pressure broadening parameter. The Elsasser narrow band model has applicability to carbon dioxide, and the maximum absorption coefficient is obtained in analytical form. From this model, the maximum nondimensional absorption coefficient within the band required in the limits in equation (1) is considered to be approximated as

$$\kappa_{\max} = \frac{R}{(1-\mathrm{e}^{-B})}\frac{\sinh(2\pi B)}{\cosh(2\pi B) - 1}. \qquad (3)$$

Equations (1) can be analytically inverted to provide an explicit formulation for the absorption coefficient as

$$\kappa = \begin{cases} \mathrm{e}^{[g_{\mathrm{wb}}(\kappa) - W(B,R)]\ln(R) + 2\mathrm{e}^{-B/4}} \\ \quad \text{for } 0 \leqslant g_{\mathrm{wb}}(\kappa) \leqslant 1 + W(B,R) - \dfrac{2\,\mathrm{e}^{-B/4}}{\ln(R)} \\ R\left[[1 + W(B,R) - g_{\mathrm{wb}}(\kappa)]\dfrac{\ln(R)}{2\,\mathrm{e}^{-B/4}}\right]^{-2} \\ \quad \text{for } 1 + W(B,R) - \dfrac{2\,\mathrm{e}^{-B/4}}{\ln(R)} < g_{\mathrm{wb}}(\kappa) \leqslant 1.0. \end{cases} \qquad \text{(4a–b)}$$

Equations (1) and (4) represent the proposed wide band formulation which has been shown to yield good results for the water vapor bands [23].

2.2. Multiple band formulation

The cumulative distribution function for spectral intervals characterized by the presence of distinct and separate dominant rotational–vibrational transitions can be modeled [22] as

$$g_{\mathrm{wb}}(k) = \sum_{i=1}^{N_{\mathrm{t}}} \frac{\Delta v_i}{\Delta v} g_i(k) \qquad (5)$$

where N_{t} is the number of dominant transitions within the spectral interval considered Δv. The transition i is dominant on the spectral interval Δv_i and is characterized by the cumulative distribution functions $g_i(k)$. Equation (5) assumes that the distinct transitions are independent and nonoverlapping. It is noted that the individual spectral intervals Δv_i may not be constant for all gas conditions (pressure, temperature and/or concentration). This work develops a simple expression for $\Delta v_i/\Delta v$ as a function of temperature which is considered to be the dominant parameter within this ratio. The fundamental assumption of the wide band model employed here is the exponential variation of the intensity-to-spacing ratio s. Thus, from the band-head or band-center, the average intensity-to-spacing ratio decreases exponentially towards the band wings. The spectral variation of s depends on the bandwidth parameter ω, which varies with respect to temperature as

$$\omega(T) = \omega_0 \sqrt{\frac{T}{T_0}} \tag{6}$$

where ω_0 is the bandwidth parameter at $T_0 = 100$ K. Considering two distinct distributions characterized by maximum values of the line intensity-to-spacing ratio $s_{\max,1}$ and $s_{\max,2}$, the ratio $\Delta v_1/\Delta v$ results from simple spectral considerations as

$$\frac{\Delta v_1}{\Delta v} = \begin{cases} 0 \\ \quad \text{for} \sqrt{\frac{T}{T_0}} \ln\left(\frac{s_{\max,1}}{s_{\max,1}}\right) \leqslant -\frac{\Delta v}{\omega_{0,2}} \\ \dfrac{\sqrt{\frac{T}{T_0}} \ln\left(\frac{s_{\max,1}}{s_{\max,2}}\right) + \frac{\Delta v}{\omega_{0,2}}}{\Delta v \left(\frac{1}{\omega_{0,1}} + \frac{1}{\omega_{0,2}}\right)} \\ \quad \text{for} -\frac{\Delta v}{\omega_{0,2}} < \sqrt{\frac{T}{T_0}} \ln\left(\frac{s_{\max,1}}{s_{\max,2}}\right) < \frac{\Delta v}{\omega_{0,1}} \\ 1 \\ \quad \text{for} \frac{\Delta v}{\omega_{0,1}} \leqslant \sqrt{\frac{T}{T_0}} \ln\left(\frac{s_{\max,1}}{s_{\max,2}}\right) \end{cases} \tag{7a–c}$$

by assuming that the spectral interval Δv_1 ends at the location where the two transitions have the same value of the minimum line intensity-to-spacing ratio $s_{\min,1} = s_{\min,2}$. The second distribution is dominant in the remaining domain of the spectral interval, $\Delta v_2 = \Delta v - \Delta v_1$. It is noted that in general, the neighboring transitions 1 and 2 are characterized by large ratios $s_{\max,1}/s_{\max,2}$. For example, if $s_{\max,1}/s_{\max,2} > 1$, as the temperature and the bandwidth parameter increase, the ratio $\Delta v_1/\Delta v$ increases, eventually becoming equal to unity for the temperature where $s_{\min,1} = s_{\max,2}$ in equation (7b). This is the minimum temperature for which the band can be accurately regarded as a single band, and equation (4) can be appropriately used. It is noted that equations (7) are only approximate, the interactions between different bands being difficult to quantify. However, the application of this model to different bands of carbon dioxide and presented below proves to be accurate. Equations (7) can be extended to more than two transitions, and it is assumed that the validity of the formulation will be diminished due to the additional approximations involved. Equations (1), (5) and (7) are used to model the two multiple bands of carbon dioxide (the 2.7 and 4.3 μm bands).

Figure 2 presents the absorption coefficient cumulative distribution function for the 2.7 μm band over the spectral interval 3300–3800 cm^{-1}, for a temperature of 500 K and pure carbon dioxide with pressures between 0.01 and 10.0 atm. The results are obtained with the more complete, multiple wide band model in equations (1), (5) and (7), as well as with the line-by-line results [1, 2]. The two transitions considered in equation (5) have band parameters with magnitudes presented in Table 1. For simplicity, the temperature and pressure variation of these band parameters is considered to be the same, determined for the strong band from Edwards [11]. The results in Fig. 2 show that the absorption coefficient distribution is accurately described by the proposed model. The smaller values of the absorption coefficient, which cannot be accurately described by the existing wide band formulations [18, 19, 23], are in good agreement with benchmark results. The improvement in the absorption coefficient distribution function is clearly illustrated by the reduction of the errors between the benchmark and the model, and is presented below.

Figure 3 presents the absorption coefficient distribution function for the 4.3 μm band, using the more complete multiple band model, for a spectral interval between 1950 and 2400 cm^{-1}, for a temperature of 500 K and the same pressures as above. The participating transitions in equation (5) have band parameters with magnitudes presented in Table 1. As in Fig. 2, the temperature and pressure variation of these parameters is considered to be the same for both bands, determined for the strong band from Edwards [11]. Although there are three participating vibrational transitions within the considered spectral interval, the accuracy of the 4.3 μm band is similar to the 2.7 μm band in Fig. 2. This aspect is discussed below in terms of errors between the benchmark calculations and the model.

This discussion shows that the multiple band spectral intervals are more difficult to model. Equations (7) show that the bands can be regarded as multiple transition bands for lower temperatures and single transition bands for high temperatures. The application of equations (1), (5) and (7) has the disadvantage of not providing an explicit expression for the absorption coefficient. Since a primary purpose of this work is to develop a simplified cumulative distribution function for use in high temperature applications, emphasis is placed on developing

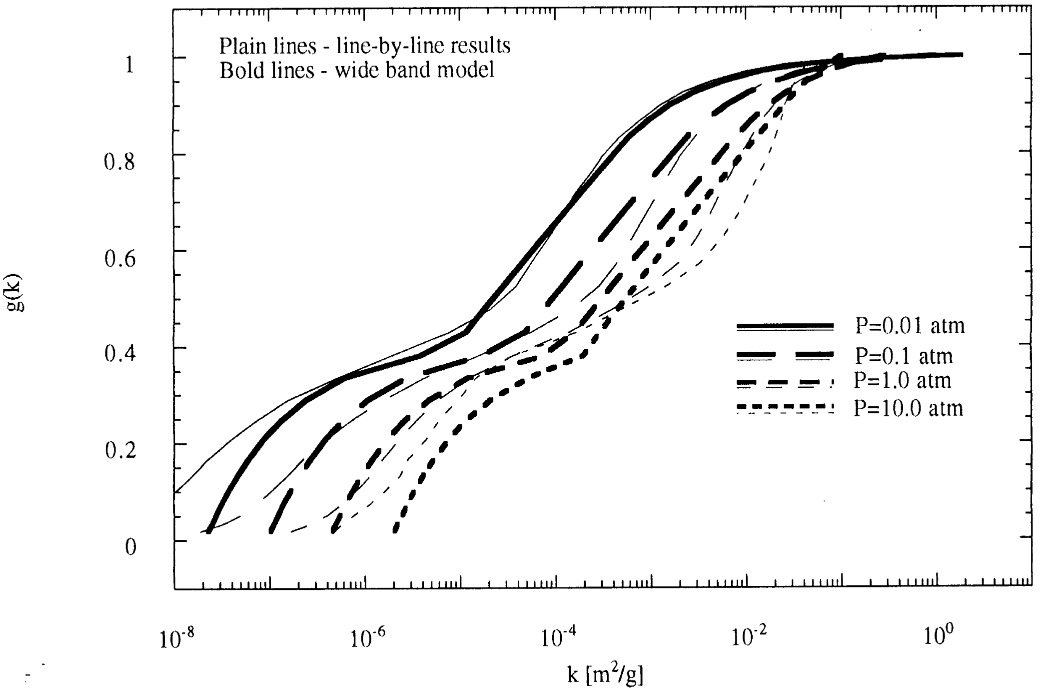

Fig. 2. Absorption coefficient cumulative distribution function for the 2.7 μm band of carbon dioxide for a temperature $T = 500$ K and for different pressures. The plain lines represent the line-by-line results [1, 2], the bold lines represent the multiple band model expressed by equations (1), (5) and (7).

Table 1
The carbon dioxide band parameters for use in equations (4) for all bands, and for use in equations (1), (5) and (7) for the 4.3 and 2.7 μm bands

Band [μm]	ν_l [cm^{-1}]	ν_u [cm^{-1}]	Transition	$\alpha_0{}^a$ [cm^{-1} g^{-1} m^2]	$\beta_0{}^{a,b}$	$\omega_0{}^a$ [cm^{-1}]
2.0	4700	5250	2, 0, 1	0.084	0.017	61.0
2.7	3300	3800	1, 0, 1	4.3	0.040	22.1
			$\Delta\nu_1{}^c$	4.3^c	0.040^c	22.1^c
			$\Delta\nu_2{}^c$	0.2^c	1×10^{-4c}	40.0^c
4.3	1950	2400	0, 0, 1	117.0	0.102	11.7
			$\Delta\nu_1{}^c$	105.3^c	0.102^c	10.5^c
			$\Delta\nu_2{}^c$	0.045^c	0.0030^c	10.8^c
9.4	1000	1125	0, −2, 1	3.4×10^{-9}	0.025	20.0
10.4	850	1000	−1, 0, 1	2.58×10^{-9}	0.0210	30.0
15.0	450	850	0, 1, 0	12.3	0.042	15.2

[a] Use with temperature and pressure dependencies in ref. [11].

[b] For all bands, $b_B = 1.3$, $n = 0.65$ for the 2.0 and 2.7 μm bands, $n = 0.7$ for the 15.0 μm band, and $n = 0.8$ for the other bands, for use in P_e. $T_0 = 100$ K and $P_0 = 1$ atm.

[c] To be used with equations (1), (5) and (7), and shown in Figs 2 and 3.

band parameters for the explicit expression of the absorption coefficient in equations (4). It is shown below that the multiple band model improves the accuracy of the absorption coefficient distribution for wide spectral intervals where several transitions are dominant on adjacent subintervals, yet the model is more computationally involved and to date no explicit formulation of the absorption coefficient has been derived. Further improve-

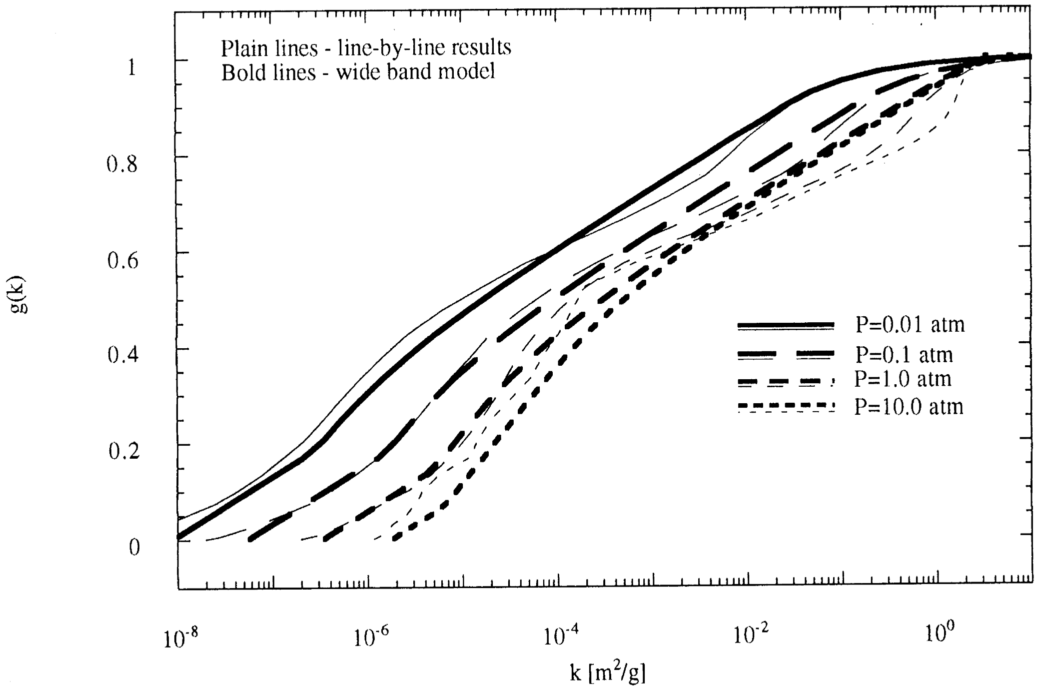

Fig. 3. Absorption coefficient cumulative distribution function for the 4.3 μm band of carbon dioxide for a temperature $T = 500$ K and for different pressures. The plain lines represent the line-by-line results [1, 2], the bold lines represent the multiple band model expressed by equations (1), (5) and (7).

ments to this model are necessary to make it easily applicable.

3. g-Function parameters for CO_2

This work develops band parameters for the six dominant bands of carbon dioxide using the model expressed in equations (4). These parameters are obtained by minimizing the differences between the cumulative distribution functions described by equations (4) and line-by-line results. Extensive comparisons between the different databases available [1, 2, 8] show that, for the dominant bands of carbon dioxide, the results are generally in good agreement for a wide range of pressures and temperatures. Some differences between existing databases occur for the weaker bands of carbon dioxide at higher temperatures. The literature indicates that the 4.3 and 2.7 μm bands are extensively studied both theoretically and experimentally [6, 7] over a large range of temperatures. The experimental data available for the other carbon dioxide bands is limited. Parker et al. [24] and Esplin and Hoke [25] present high temperature (up to 800 K) measurements for the 12 μm window region, including the 15.0, 10.4 and 9.4 μm bands. The results show good agreement between the experimental data and the HITEMP database. Based upon these experimental results, this work develops band parameters from the line-by-line database [1, 2], for temperatures up to 1000 K. The results for the 4.3 and 2.7 μm bands are then compared with the narrow band database [8, 9] for elevated temperatures. The absence of reliable line-by-line data for high temperature applications, together with the computational efficiency and accuracy of the narrow band data justify this procedure. For all calculations, a thorough comparison with the results of Edwards [11–15] is performed.

Wide band parameters are generated by minimizing the differences between the wide band absorption coefficient cumulative distribution functions obtained with the benchmark database and the proposed model. The spectral lower limit ν_l, upper limit ν_u and the spectral interval $\Delta\nu = \nu_u - \nu_l$ are set for each band and maintained for all pressures and temperatures. The band spectral limits are presented in Table 1. The choice for the spectral limits is in most cases provided by the line-by-line results. This procedure is different from the original formulation of the wide band model, where the band limits are not specifically required. The original wide band model calculates the wide band absorption, which for a given pathlength becomes independent of the band spectral magnitude. The proposed model attempts to determine specific values of the absorption coefficient within the band, and is dependent upon the spectral interval considered. As the spectral interval widens, the corresponding distribution function shifts towards smaller values of the absorption coefficient. The original wide band parameters describing the band intensity α [11, equation (73)], the bandwidth parameter ω [11, equation (95)] and the broadening parameter β [11, equation (99)] are altered to more accurately describe the absorption coefficient cumulative distribution function. The broadening parameter β is used to calculate the pressure broadening parameter $B = \beta P_e$, where P_e is the effective pressure [11, equation (58)]. Note that Edwards [11] uses a pressure broadening parameter that is π times the pressure broadening parameter B used here. It is noted that the temperature and pressure variations of the above band parameters follow the recommendations of Edwards [11].

Initially, the cumulative distribution functions for temperatures between 300, 500, 700, 900 and 1000 K are calculated for the 2.0, 2.7, 4.3, 9.4, 10.4 and 15.0 μm bands. For all considered bands, pure carbon dioxide with pressures of 0.01, 0.1, 1.0 and 10.0 atm is considered. For each distinct cumulative distribution function, 32 values of the absorption coefficient corresponding to the Gaussian quadrature locations are obtained. The root mean square (RMS_k) of the differences defined as

$$\delta_k = \frac{k_e - k_m}{k_e} \tag{8}$$

is calculated for the different distributions, where k_e is the absorption coefficient for the benchmark calculations [1, 2, 8] and k_m is the absorption coefficient for the proposed model [equations (4)] for the same set of temperatures and pressures and values of the cumulative distribution function. The band parameter development process minimizes the differences expressed in equation (8) for $g(\kappa) > 0.2$ and for the range of temperatures noted above and pressures between 0.1 and 10.0 atm. This choice of pressure results from the fact that the exponential band model was primarily designed to calculate the radiative transfer at atmospheric pressures [11]. The wide band parameters for carbon dioxide originally developed by Edwards are primarily based upon measurements up to 1390 K and for a total pressure range between 0.5 and 10 atm [26]. The calculations below discuss the accuracy of the band model for lower total pressures. The RMS_k is calculated using absorption coefficients corresponding to $g(k)$ greater than 0.2. This procedure is justifiable by noting that $g(k) < 0.2$ there correspond relatively small values of the absorption coefficient that are physically of less importance for most engineering applications. In addition, the small absorption coefficient region of the cumulative distribution function originates primarily in the band wings, which are not exhaustively studied to date, particularly for high temperatures.

Table 1 shows the values of the suggested band parameters, for the wide bands considered. Although slightly different, all the values proposed are of a similar order of magnitude with the original parameters developed by Edwards [11]. Table 1 presents band parameters for use with equations (4) for all bands. Band parameters are also recommended for the 2.7 and 4.3 μm bands for use with the more complete, multiple band model in equation (5). The band parameters presented in Table 1 are then used to calculate differences between the model and the benchmark calculations. Thus, Table 2 presents values of $\mathrm{RMS}_{k,\mathrm{lbl}}$ for a temperature interval of 300–1000 K for the 2.0, 2.7, 4.3, 9.4, 10.4 and 15.0 μm bands with the line-by-line database as benchmark. The $\mathrm{RMS}_{k,\mathrm{nb}}$ for the 2.7 and 4.3 μm bands considers distributions with temperatures from 300 K and up to 2900 K in increments of 200 K. These reported results consider the narrow band database [8] as benchmark. The more complete model in equation (5) is also applied to the 2.7 and 4.3 μm bands, using the band parameter in Table 1, and compared to the line-by-line calculations for temperatures up to 1000 K ($\mathrm{RMS}_{k,\mathrm{c,lbl}}$). The same procedure applies to the wide band absorption (RMS_A) results discussed below.

Figures 4–9 present the cumulative distribution functions for the investigated bands, using the proposed model expressed by equations (4) and benchmark results. All figures present the absorption coefficient distribution functions from the line-by-line database [1, 2], the narrow band database [8] and the wide band model in equations (4), for temperatures of 500 and 1000 K. Additionally, the results for the 2.7 μm band (Fig. 5) and the 4.3 μm band (Fig. 6) present the wide band model and the narrow band base results for temperatures of 1500 K and 2500 K.

Figure 5 shows the absorption coefficient cumulative distribution function for temperatures of 500, 1000, 1500 and 2500 K, and for pressures of 0.01–10 atm, for the 2.7 μm band. The results in Fig. 5 show that for low temperatures the model introduces relatively large differences in the low absorption coefficient regions. As the temperature increases, noticeable differences occur for small values of the pressure. The behavior at low temperatures is attributed to the interaction between different rotational–vibrational transitions as indicated in Fig. 2. At low temperatures the spectral interval are more accurately modeled as a multiple band, while at high temperatures there remains a single dominant transition over the entire spectral interval considered. Table 2 shows that the $\mathrm{RMS}_{k,\mathrm{c,lbl}}$ values for the 2.7 μm band are reduced by around 40% when the multiple band model is employed as compared to $\mathrm{RMS}_{k,\mathrm{lbl}}$ for the same band and same temperature range. The reduction is about one order of magnitude, when only temperatures up to 700 K are considered, and the calculation includes the entire distribution function, $0.0 < g(k) < 1.0$, since the multiple band model is designed to more accurately describe the

Table 2
Root mean square errors for the absorption coefficient cumulative distribution function (RMS_k) and the wide band absorption (RMS_A). All $g_{wb}(k)$ parameters from Table 1. Absorption coefficient cumulative distribution function error include $g_{wb}(k) > 0.2$

Band [μm]	$\mathrm{RMS}_{k,\mathrm{lbl}}$ [%]	$\mathrm{RMS}_{k,\mathrm{nb}}$ [%]	$\mathrm{RMS}_{k,\mathrm{c,lbl}}$ [%]	$\mathrm{RMS}_{\mathrm{A,lbl}}$ [%]	$\mathrm{RMS}_{\mathrm{A,nb}}$ [%]	$\mathrm{RMS}_{\mathrm{A,c,lbl}}$ [%]	$\mathrm{RMS}_{\mathrm{A,edw}}$ [%]
2.0	37.4	—	—	9.6	—	—	18.2
2.7	92.9	74.5	52.6	10.3	13.6	9.6	12.3
4.3	87.5	75.5	50.4	7.6	10.7	9.8	7.3
9.4	33.3	—	—	9.1	—	—	18.7
10.4	31.2	—	—	12.9	—	—	22.8
15.0	32.3	—	—	5.9	—	—	15.2

lbl = line-by-line database for temperatures in the range 300–1000 K, pressures in the range of 0.1–10.0 atm. RMS_A used lengths in the range 10^{-3}–10^3 meters.
nb = narrow band database for temperatures in the range 300–2900 K, pressures in the range of 0.1–10.0 atm. RMS_A used lengths in the range 10^{-3}–10^3 meters.
c = more complete model in equations (7) with parameters in Table 1.
edw = Edwards [11] results for temperatures in the range 300–2900 K, pressures in the range of 0.1–10.0 atm and lengths in the range 10^{-2}–10^3 m.

lower regions of the cumulative distribution function. Figure 5 shows that the narrow band database and the line-by-line database are in relatively good agreement for the 2.7 μm band.

Figure 6 shows the 4.3 μm band for the same temperatures and pressures as Fig. 5. The model in equations (4) accurately predicts the actual absorption coefficient cumulative distribution functions for most of the cases presented. The largest differences occur at elevated temperatures, for small values of the absorption coefficient, where the model overpredicts the actual distributions. This band is dominated by three different rotational–vibrational transitions at low temperatures, while as the temperature increases, the weaker transitions centered in the vicinity of 4.8 and 5.2 μm are incorporated by the strong transition having the head located near 4.3 μm. The employment of the more complete, multiple band model in equations (1), (5) and (7) and shown in Fig. 3 reduces the RMS_k by around 40% for the considered temperature and pressure intervals. The reduction is similar to the 2.7 μm spectral interval, although there are three rotational–vibrational bands over the considered spectral interval, while only two are accounted for in Fig. 3. The narrow band database and the line-by-line database are in relatively good agreement.

Finally, the weaker bands are the 2.0, 9.4, 10.4 and 15.0 μm bands. The absorption coefficient distribution function for temperatures of 500 and 1000 K and pressures between 0.01 and 10.0 atm are presented for these bands in Figs 4, 7, 8 and 9. The results in the top portion of each figure show that the two databases are in very good agreement at 500 K, yet noticeable differences occur in the bottom portion of each figure at 1000 K. The expected increase in values of the absorption coefficient with temperature that is observed in the line-by-line database supports the use of this database as the benchmark for the wide band model parameters determination. All these bands are accurately predicting the benchmark results over the entire temperature and pressure intervals considered.

Table 2 shows the RMS_k error introduced by the wide band model when compared to the benchmark results, for each individual band, for values of the cumulative distribution function $g(k) > 0.2$. The 2.0, 9.4, 10.4 and 15.0 μm bands are characterized by similar values of the RMS_k. The spectral intervals of the 4.3 and 2.7 μm bands are dominated by different transitions, particularly for lower temperatures. This explains the larger values of the RMS_k for these bands. The complete band model described in equation (5) improves the accuracy of the absorption coefficient distribution function, for these bands. Note that the errors based upon the entire cumulative distribution function will be significantly higher, mainly due to more substantial differences in the small regions of the distribution functions, physically of limited importance.

4. Wide band absorption comparisons

The band model developed above can be used to calculate the gas absorption over specified spectral intervals. The wide band absorptivity is defined as

$$A^* = \frac{A}{\omega} = \frac{1}{\omega}\int_{\Delta\nu}(1-e^{-k(\nu)u})\,\mathrm{d}\nu = \frac{\Delta\nu}{\omega}\int_0^1(1-e^{-ku})\,\mathrm{d}g \tag{9}$$

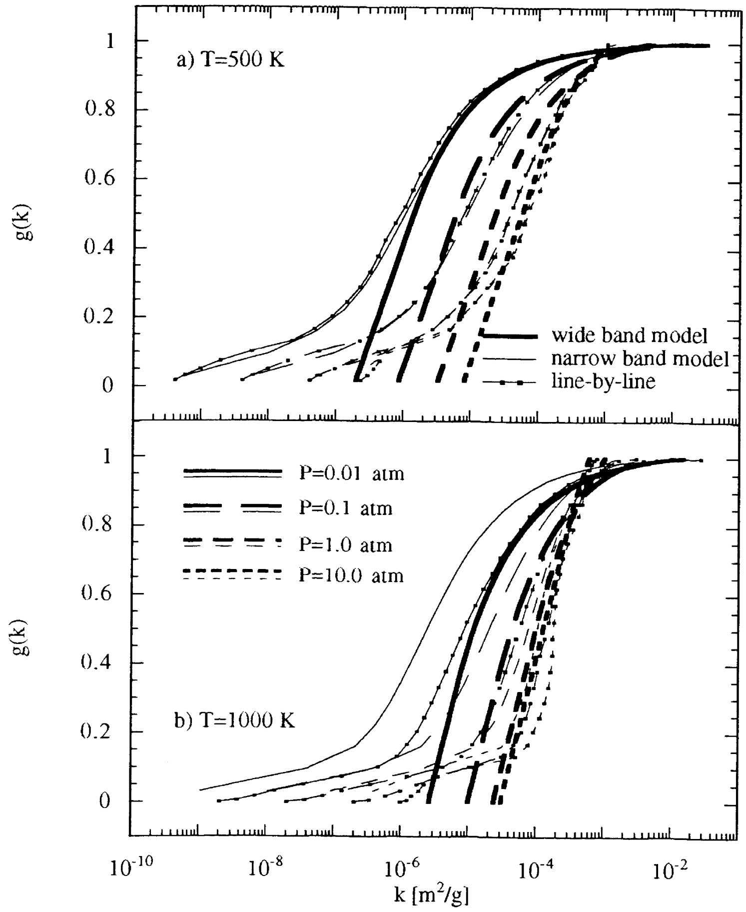

Fig. 4. Absorption coefficient cumulative distribution function for the 2.0 μm band of carbon dioxide, for (a) $T = 500$ K and (b) $T = 1000$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

where $\Delta\nu$ is the wide band spectral interval and u is the mass pathlength, $u = \rho L$, defined as the product between the absorbing gas density ρ and the optical length L. This last integral is evaluated by

$$A^* = \frac{\Delta\nu}{\omega}\sum_{i=1}^{N_q}(1-e^{-k_i u})w_i \tag{10}$$

where N_q is the number of quadratures of the summation, w_i are the weights and k_i are the corresponding absorption coefficients.

The proposed model and the band parameters developed above are applied to the different bands of carbon dioxide. The number of quadratures $N_q = 32$ is used for the following calculations. It is noted that as B increases, the number of quadratures can be decreased. Alternatively, a different integration scheme with a reduced number of quadratures can be considered (Soufiani and Taine [8]). The same ranges for temperature and pressure as above are used to evaluate the band absorption, for pathlengths between 10^{-3} and 10^3 m. Equation (10) is applied to the model described by equations (4) and compared to the results obtained with benchmark calculations in the same manner as for the absorption coefficient distribution functions. The mean root square error $\mathrm{RMS_A}$ of the differences

$$\delta_A = \frac{A_e^* - A_m^*}{A_e^*} \tag{11}$$

is calculated for each band for the values of temperature, pressure and optical length indicated above. A_m^* are calculated using equations (4) together with the band parameters in Table 1 and A_e^* are obtained from line-by-line, narrow band model or Edwards wide band model calculations.

Table 2 shows the root mean square error for the wide band absorption ($\mathrm{RMS_A}$), for temperatures in the ranges

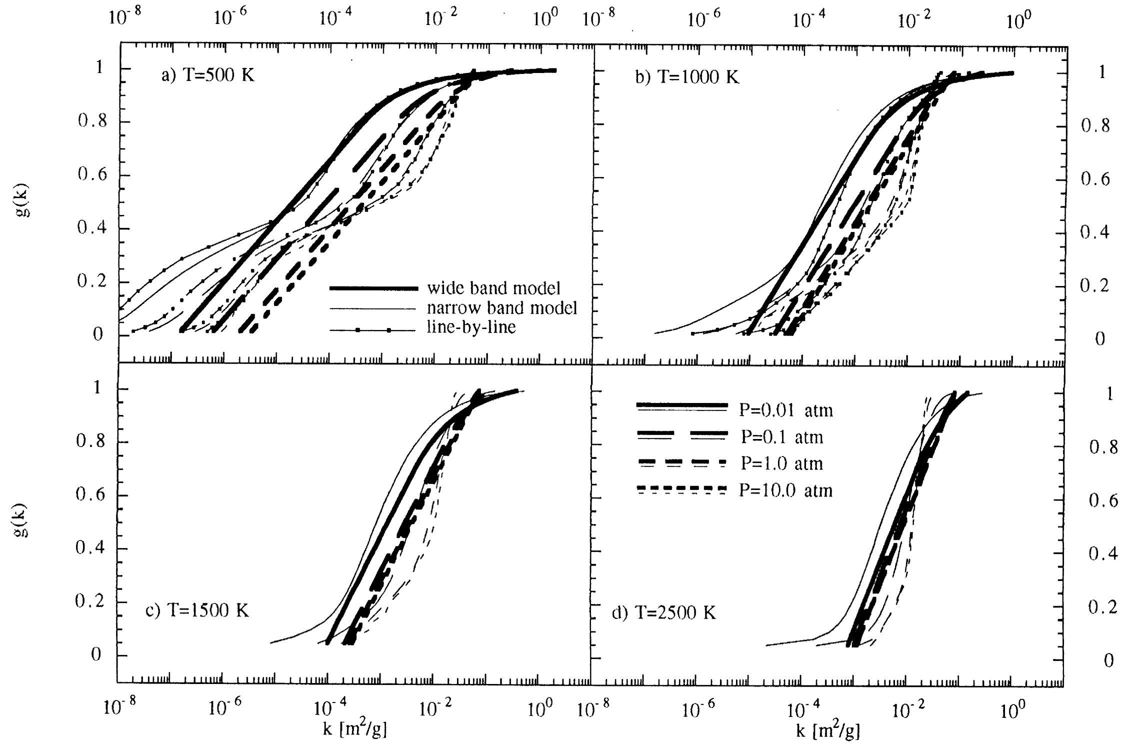

Fig. 5. Absorption coefficient cumulative distribution function for the 2.7 μm band of carbon dioxide, for (a) $T = 500$ K, (b) $T = 1000$ K, (c) $T = 1500$ K and (d) $T = 2500$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

300–1000 K for all bands compared to line-by-line database ($\mathrm{RMS}_{\mathrm{A,lbl}}$), and 300 K through 2900 K for the 2.7 and 4.3 μm bands as compared to the narrow band database ($\mathrm{RMS}_{\mathrm{A,nb}}$) for the pressure range of 0.1 through 10 atm. The $\mathrm{RMS}_{\mathrm{A,lbl}}$ is 7.6% for the strongest carbon dioxide band centered at 4.3 μm. The 2.0, 2.7, 9.4 and 15.0 μm bands yield $\mathrm{RMS}_{\mathrm{A,lbl}}$ values below 10%, and the 10.4 μm band yields 12.9%. The multiple band model employed for the 2.7 and 4.3 μm bands yields same order values for $\mathrm{RMS}_{\mathrm{A,c,lbl}}$ as $\mathrm{RMS}_{\mathrm{A,lbl}}$. The analysis of $\mathrm{RMS}_{\mathrm{A,nb}}$ shows that the 2.7 and 4.3 μm bands yield 13.6 and 10.7%, respectively.

Table 3 presents the average differences $\bar{\delta}_{\mathrm{A}}$ between the wide band absorption resulted from the proposed model in equations (4) and the benchmark calculations. The results in Table 3 include two different pathlengths, namely 10^{-3}–10^{3} m and 10^{-1}–10^{3} m, respectively. This choice illustrates the larger differences observed for very small pathlengths, corresponding to small values of band absorption. This aspect is observed by numerous publications [16, 17, 20]. The top four rows of Table 3 present the average differences for specific values of temperatures and for specific pathlength ranges, over the considered pressure range of 0.1–10.0 atm. The differences are calculated using the line-by-line results for temperatures of 500 and 1000 K for all bands, and the narrow band results at 1500 and 2500 K for the 2.7 and 4.3 μm bands. The results show that the strongest band of carbon dioxide (4.3 μm band) is accurately described by the proposed model, with differences of up to 11% for the 10^{-3}–10^{3} meter pathlength range, and 7.7% for the 10^{-1}–10^{3} meter range for the temperatures considered. The 2.0, 2.7, 9.4, 10.4 and 15.0 μm bands introduce differences with respect to the line-by-line database of up to 13% for the 10^{-3}–10^{3} meter pathlength range, and 11% for the 10^{-1} to 10^{3} meter pathlength range, but generally the differences are below 8%. The differences for the two pathlength ranges considered are relatively close in most cases which indicates the good accuracy of the model for small optical paths.

The bottom four rows of Table 3 show the differences between the proposed model and the benchmark calculations for specific pressures for the considered pathlength ranges. The differences are averaged over the temperature range between 300 and 1000 K for all the bands, with the line-by-line database as benchmark. The results show that the differences are larger for a pressure of 0.01 atm for all bands except the strong 4.3 μm band,

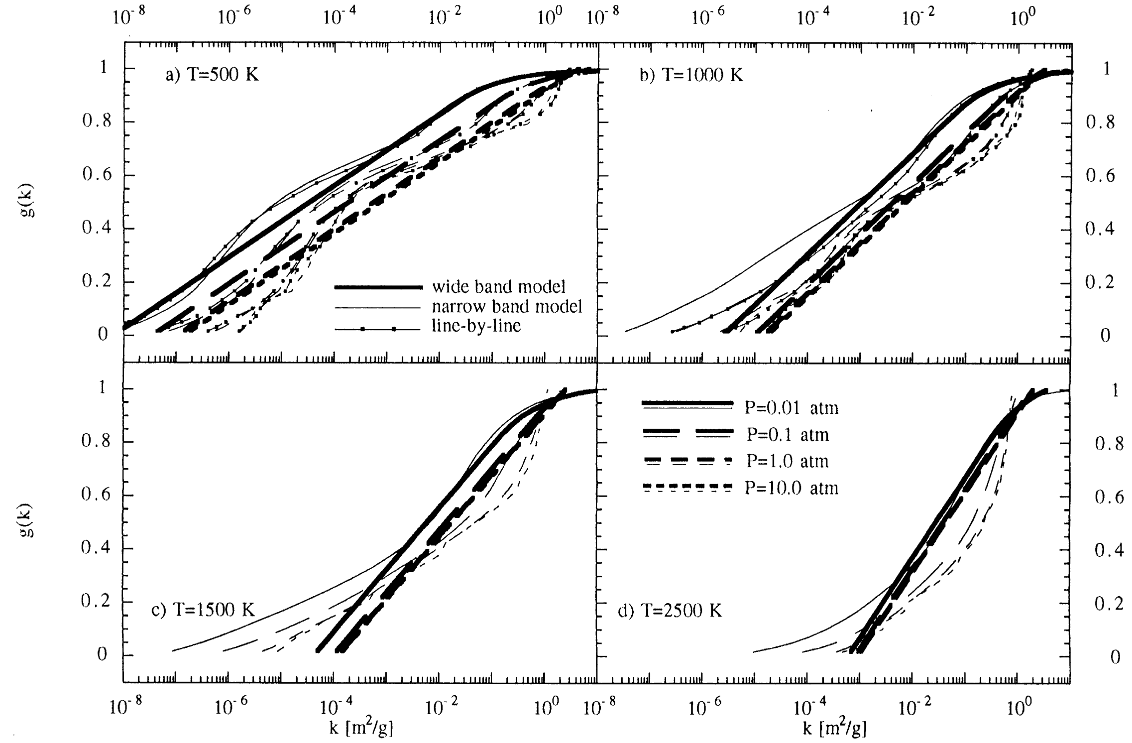

Fig. 6. Absorption coefficient cumulative distribution function for the 4.3 μm band of carbon dioxide, for (a) $T = 500$ K, (b) $T = 1000$ K (c) $T = 1500$ K and (d) $T = 2500$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

for which the differences are below 9%. For pressures 0.1 atm and higher, the differences are below 11% for all bands, relatively constant for all values of pressure, showing the consistency of the model. The results are not significantly different for the two different pathlengths considered.

A comparison between the wide band absorption results obtained with the proposed model [equations (4)] together with the band parameters in Table 1, and the results obtained using Edwards [11] correlations is performed and presented in Table 2 ($\mathrm{RMS}_{\mathrm{A,edw}}$). The $\mathrm{RMS}_{\mathrm{A}}$ between the wide band absorption predicted by the two models varies from a minimum of 7.3% for the 4.3 μm band to a maximum of 22.8% for the 10.4 μm band, for a temperature range between 300 and 2900 K and a pressure range between 0.1 and 10 atm of pure carbon dioxide, for pathlengths between 0.01 and 10 m. It is noted that, except for the 4.3 and 2.0 μm bands, the differences between this model and Edwards results occur primarily for elevated temperatures, for which there is little accurate experimental validation. It is concluded that the proposed model expressed by equations (4) accurately describes the carbon dioxide rotational–vibrational bands, for a wide range of temperatures and pressures. Improvements in the existing high temperature information for the weaker bands may contribute to future enhancements in the wide band parameters for these bands.

5. Conclusions

This work applies a model for the absorption coefficient cumulative distribution function for large spectral intervals, corresponding to entire rotational–vibrational bands for carbon dioxide. The model is exact in the gas pressure limits and it is approximate for intermediary values of the gas pressure. The model explicitly expresses the absorption coefficient as a function of the wide band cumulative distribution function and thus simplifies the solution of the radiative transfer equation. The model accurately describes the absorption coefficient distribution for wide spectral intervals, with larger differences occurring for relatively small absorption coefficients corresponding to the band wings.

Band parameters for the most important rotational–vibrational bands of carbon dioxide are developed. This work preserves the variation of the band parameters with

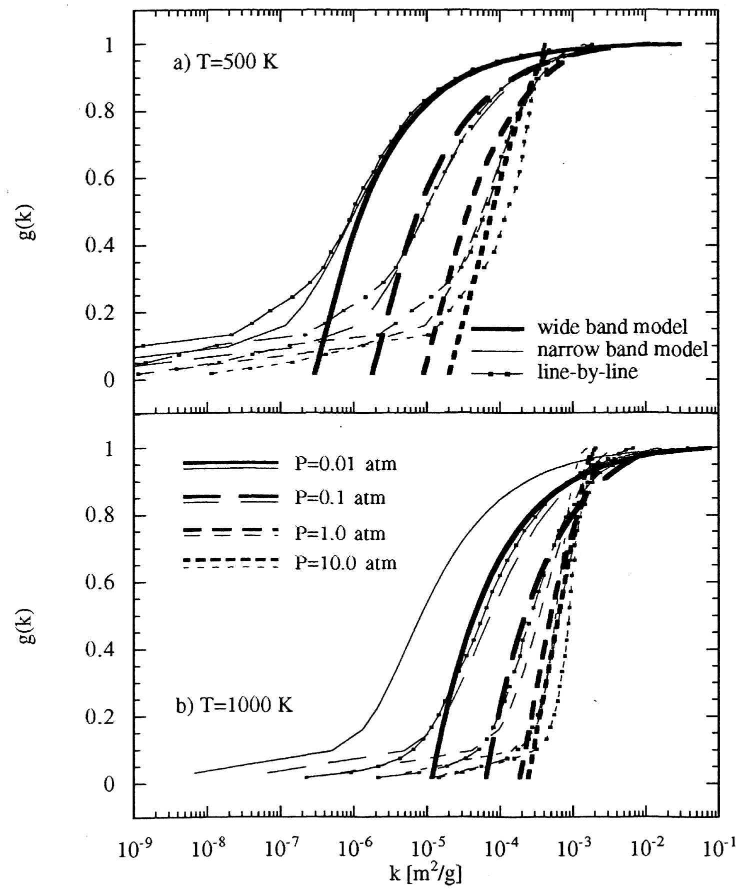

Fig. 7. Absorption coefficient cumulative distribution function for the 9.4 μm band of carbon dioxide, for (a) $T = 500$ K and (b) $T = 1000$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

respect to pressure and temperature as prescribed by Edwards [11, 12], and adjusts the wide band parameters in order to accurately represent the absorption coefficient cumulative distribution function. In order to determine the effective absorption coefficient distribution functions, important for calculations in nonhomogeneous media, the model introduces spectral boundaries for the considered bands that are maintained constant for all conditions. The proposed parameters result from comparisons with existing databases, namely the line-by-line database [1, 2] an the narrow band database [8]. The results show that the model accurately predicts the absorption coefficient cumulative distribution function for the most important rotational–vibrational bands.

The model is applied to calculate the wide band absorption and compares the equivalent results from the benchmark databases and from Edwards [11–15]. The results are in good agreement with the benchmark calculations for most cases, with larger differences occurring for small pressures, where the absorption is very small. The band absorption results are generally within 10% of benchmark results for pressures in the range between 0.1 and 10 atm.

The proposed model together with the recommended band parameters can be used for accurate transport calculations over large spectral intervals for carbon dioxide in both homogeneous and nonhomogeneous media. Such an absorption coefficient model is also important in problems involving particle scattering. The explicit expressions of the absorption coefficient reduce the computational burden in the solution of the radiative transfer equation. Future work will be required to consider improved variations of the band parameters with pressure and temperature, as new high temperature experimental data and line-by-line results are reported.

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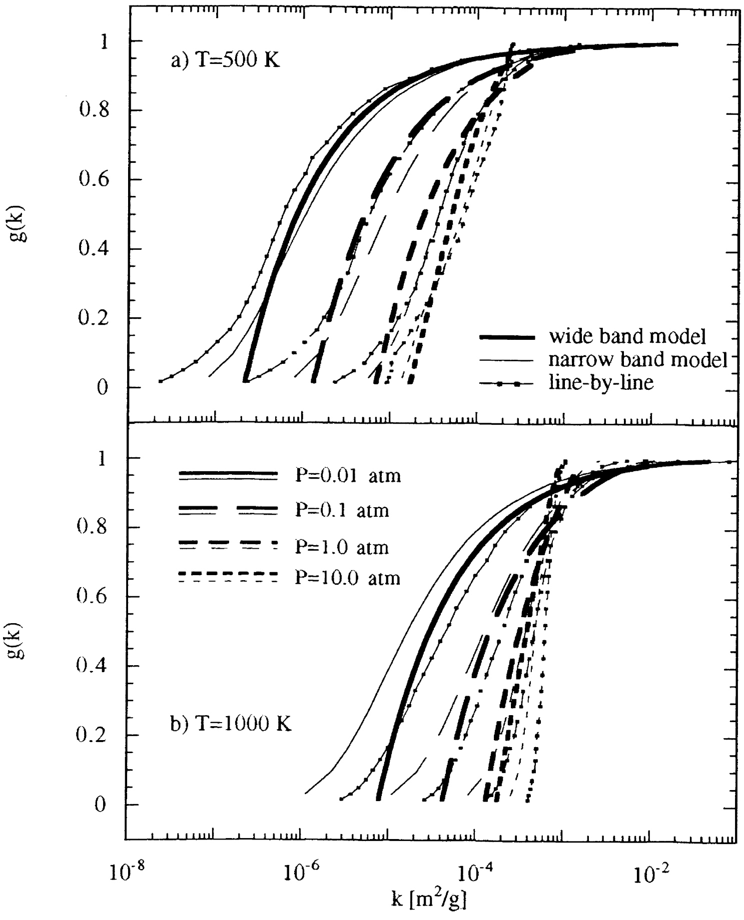

Fig. 8. Absorption coefficient cumulative distribution function for the 10.4 μm band of carbon dioxide, for (a) $T = 500$ K and (b) $T = 1000$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

Table 3
Average difference of the wide band absorption for the carbon dioxide bands, between the wide band model in equations (4) and the line-by-line data base [1, 2] for all the bands, and between the wide band model [equation (4)] and the narrow band data base [8] for the 2.7 and 4.3 μm bands for the 1500 and 2500 K cases. Rows 1–4 present the results for the indicated temperatures and range of pathlengths, and for pressures in the range 0.1–10.0 atm. Rows 5–8 present the results for the indicated pressures and range of pathlengths, and for temperatures in the range 300–1000 K for all the bands

T [K] [rows 1–4] P [atm] [rows 5–8]	$\bar{\delta}_{\mathrm{A}\ 2.0\ \mu\mathrm{m\ band}}$ [%]		$\bar{\delta}_{\mathrm{A}\ 2.7\ \mu\mathrm{m\ band}}$ [%]		$\bar{\delta}_{\mathrm{A}\ 4.3\ \mu\mathrm{m\ band}}$ [%]		$\bar{\delta}_{\mathrm{A}\ 9.4\ \mu\mathrm{m\ band}}$ [%]		$\bar{\delta}_{\mathrm{A}\ 10.4\ \mu\mathrm{m\ band}}$ [%]		$\bar{\delta}_{\mathrm{A}\ 15.0\ \mu\mathrm{m\ band}}$ [%]	
	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]	10^{-3}–10^{3} [m]	10^{-1}–10^{3} [m]
$T = 500$	8.7	8.1	12.3	11.3	8.6	6.4	9.2	13.3	6.7	5.4	5.7	5.3
$T = 100$	8.9	7.4	7.9	7.2	6.4	3.7	7.6	8.7	11.1	7.5	5.0	4.3
$T = 1500$	—	—	7.8	5.3	10.5	7.7	—	—	—	—	—	—
$T = 2500$	—	—	14.3	7.18	10.7	5.4	—	—	—	—	—	—
$P = 0.01$	28.4	24.1	25.8	20.1	9.4	5.4	23.0	19.2	11.8	11.3	14.0	10.5
$P = 0.1$	8.3	8.0	9.7	10.0	5.3	4.4	8.0	8.1	8.6	8.1	7.1	8.3
$P = 1.0$	9.3	9.7	10.3	10.8	8.7	4.8	7.5	7.2	11.1	8.4	5.9	5.1
$P = 10.0$	10.0	8.7	9.2	5.9	6.1	5.0	9.6	6.9	12.5	8.0	4.3	2.9

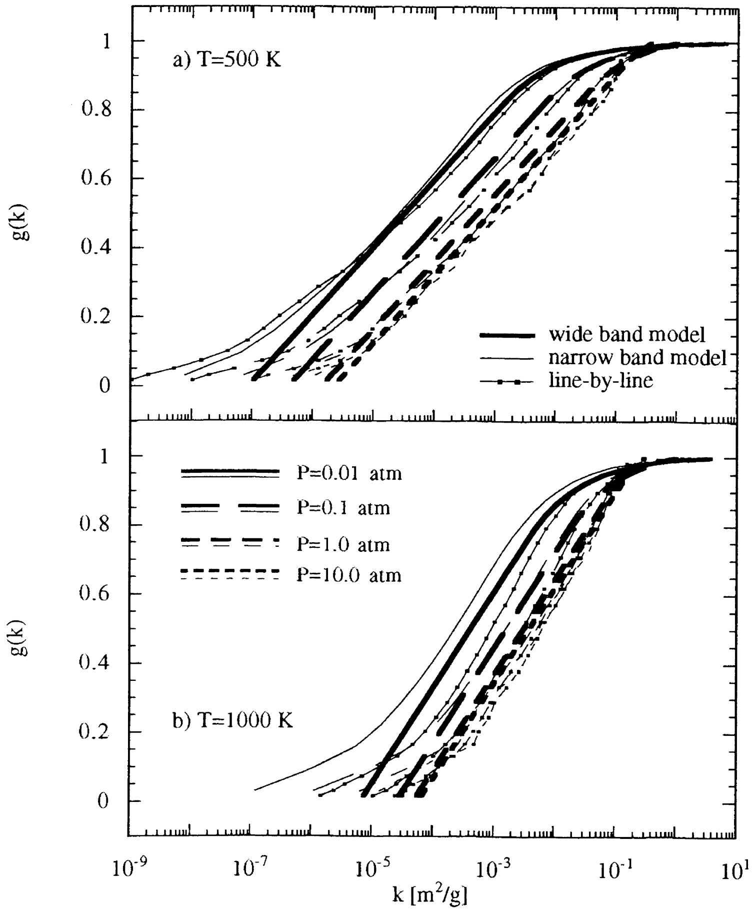

Fig. 9. Absorption coefficient cumulative distribution function for the 15.0 μm band of carbon dioxide, for (a) $T = 500$ K and (b) $T = 1000$ K, for different pressures. The bold lines represent the proposed model expressed by equations (4), the plain lines represent the narrow band model results [8] and the marked lines represent the line-by-line results [1, 2].

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