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An improved WSGGM-based narrow band model for the CO_2 4.3 μm band

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Abstract — An accurate WSGGM-based narrow band (WNB) model is investigated in the CO_2 4.3 μm band for use in inverse radiative instrumentation. The WNB model of Kim and Song is tested first with 24 gray gases for all of the narrow bands and it shows significant error compared with the line-by-line (LBL) results for two typical non-isothermal layers. A modification of this model is proposed using the concept of correlated k-distribution (CK) and assuming that the scaling approximation may be justified. With only seven gray gases taken independently for each narrow band (optimised and tabulated), this model shows less than 1 % deviation from the LBL results for most of the important narrow bands around 4.3 μm. Further extension of the WNB model is tried by applying the CK fictitious gases (CKFG) concept by taking, independently for each narrow band, three fictitious gases for each of which three gray gases are taken. This results in 3^3 gray gases which are spectrally overlapped with each other in a random fashion. Despite the complexity and labour, the test of the CKFG-based WNB model reveals greater error (a few percent or more) than the previous CK-based modification for the CO_2 4.3 μm band. Therefore, use of the CK-based WNB model for accurate and economical computations is recommended. © Elsevier, Paris.

radiation / absorption coefficient / narrow band / carbon dioxide / gray gas / fictitious gas

Résumé — Un modèle à bandes étroites amélioré pour la bande 4,3 μm du CO_2, basé sur la méthode de la somme pondérée de gaz gris. On analyse un modèle précis à bandes étroites (WNB) pour représenter la bande à 4,3 μm du CO_2. Ce modèle est basé sur la méthode de la somme pondérée de gaz gris (WSGGM) et est destiné à une application en instrumentation impliquant les méthodes inverses en rayonnement. Le modèle WNB de Kim et Song est d'abord essayé avec 24 gaz gris pour toutes les bandes étroites. Ce test révèle une erreur appréciable lorsque les résultats sont comparés avec ceux obtenus par un calcul raie par raie (LBL) pour deux couches anisothermes typiques. On propose une modification du modèle tirant parti du concept de distribution cumulée du facteur d'absorption (CK) et en supposant que l'approximation d'échelle est justifiée. Avec seulement 7 gaz gris choisis de façon indépendante pour chaque bande étroite (valeurs optimisées et mises en tableau), ce modèle conduit à des écarts de moins de 1 %, avec les résultats raie par raie (LBL) pour la plupart des bandes étroites importantes autour de 4,3 μm. On tente aussi une autre expansion du modèle WNB en appliquant le concept CK à gaz imaginaires (CKFG). On choisit, de façon indépendante pour chaque bande étroite, trois gaz imaginaires pour chacun desquels on prend trois gaz gris, ce qui résulte en 3^3 gaz gris, dont les spectres se chevauchent de façon arbitraire. Malgré sa complexité et sa difficulté de mise en œuvre, l'utilisation du modèle WNB basé sur la méthode CKFG génère une erreur supérieure (plus de 1 %) à celle obtenue avec la modification précédente de la méthode CK pour la bande 4,3 μm du CO_2. Ainsi, il est recommandé d'utiliser le modèle WNB basé sur la méthode CK: les calculs sont précis et économiques en temps de calcul. © Elsevier, Paris.

rayonnement / coefficient d'absorption / bande étroite / gaz carbonique / gaz gris / gaz imaginaire

Nomenclature

c	speed of light	$2.998 \cdot 10^8$ m·s^{-1}
E	modelling error	
E''	transition energy of a fictitious gas normalised by hc	cm^{-1}
g	cumulative k-distribution	
h	Planck's constant	$6.63 \cdot 10^{-34}$ J·s
I	radiation intensity	
k	Boltzmann's constant	$1.3806 \cdot 10^{-23}$ J·K^{-1}
L	path length	

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P pressure of medium
s co-ordinate along the radiation path
T temperature of medium
W weighting factor
Y mole fraction of species

Greek letters

α modelling constant in WSGGM-based narrow band model
ε spectral emissivity
η wavenumber
κ absorption coefficient
κ_0 modelling constant in WSGGM-based narrow band model

Subscripts

b blackbody
i index of gray gas in the first fictitious gas
j index of gray gas or in the second fictitious gas
k index of gray gas in the third fictitious gas
m modelled value
s index of species in medium
t true value or LBL value
η at a wavenumber
i, j, k index corresponding to joint weight of i'th, j'th and k'th gray gas

1. INTRODUCTION

Accurate modelling of the non-gray behaviour of gaseous mixtures is very important for treating the radiative heat transfer problems in combustion systems such as furnaces and engines, or in meteorological and astronomical areas. Efficient and accurate prediction of the radiative heat transfer in these areas remains a challenging problem due to the strong spectral variation of the absorption coefficients of emitting and absorbing species such as H_2O and CO_2.

The most accurate modelling technique is the line-by-line (LBL) approach based on a direct calculation of all radiation lines, such as has been done by Hartmann et al. [1] and Rothman et al. [2]. However, the LBL method requires not only a huge set of spectroscopic data, but also great computational efforts. In an LBL approach, for instance, the spectral computations have to be performed at about 10^6 wavenumbers to cover the entire IR spectrum range of CO_2 at high temperature, which proves too impractical to apply to real engineering problems.

Because of these difficulties, a great deal of effort has been expended in the search for alternative models of the gas radiative properties. These can be classified into three types: narrow band models, wide band models and global band models.

In narrow band models, the spectrum is subdivided into bands of tens of cm^{-1} wavenumber intervals, the width over each of which is sufficiently small to assume a constant value of the Planck function, while sufficiently wide to include a great number of absorption lines. The classical narrow band models are called statistical models, among which the Elsasser model [3] is the simplest. The Statistical Narrow-Band (SNB) model developed by Mayer and Goody [3] gives results which agree with the LBL calculations with an accuracy of about a few percent error in the case of isothermal and homogeneous columns. The SNB model requires a supplementary approximation for a non-isothermal and/or inhomogeneous medium. Many approximations have been studied by Young [4] and other workers [5], among which the Curtis Godson (CG) approximation is the most common. SNB models with the CG or other similar approximations yield satisfactory results for most industrial applications, although these methods have the following disadvantages: (1) they have relatively large error compared with LBL computations, (2) they give transmittance instead of absorption coefficient (a more versatile parameter), and (3) they require CG-like approximations for inhomogeneous media, further sacrificing the accuracy.

Goody and Young [3] propose the k-distribution method as another efficient technique. The essence of this method is to replace the spectral integration over wavenumber with the integration over the absorption coefficient to find the weighting factor distribution curve. Non-isothermal and/or inhomogeneous media may be handled using the correlated-k (CK) method, as has been studied for atmospheric applications by Goody [6], and for combustion applications by Rivière et al. [7]. The correlated-k fictitious gas (CKFG) method, an extension of the CK method, has been developed by Taine and Rivière et al. [8, 9] to palliate the major deficiency of the CK method, i.e., overestimation of spectral correlation between intense emitting lines in hot regions and intense absorbing lines in cold regions of the medium. It has been verified by Rieviere, Soufiani, and Taine [10, 11] that CK and CKFG model yield very accurate results for the spectral properties of combustion products.

For heat transfer engineers who are interested only in obtaining radiative heat fluxes over the entire spectrum, it is desirable to employ models that can readily predict the total absorption or emission. A wide band model is a useful tool for this purpose. The box model is the simplest one developed by Penner [12] in a successful application to diatomic gases, although the accuracy is very sensitive to the choice of the effective bandwidth. The exponential wide band model, first developed by Edwards and Menard [13] and further developed by Edwards and his co-workers [14, 15], is the most widely-used wide band model.

The global model is the most efficient one which can be used to predict total radiative fluxes to any accuracy. The weighted-sum-of-gray-gases (WSGG)

model, introduced by Hottel [16] and later numerically optimised by Smith et al. [17], is the most popular global model. The capability of the WSGG idea has been demonstrated for general non-isothermal/non-homogeneous media by Modest [18] and Song and Viskanta [19, 20]. The WSGG model has been improved to the spectral line-based weighted-sum-of-gray-gases (SLW) model by Denison and Webb [21–23]. Marin and Buckius [24] have made CK-based models for CO_2 and H_2O on each wide band. This modelling is either for the total spectrum or part of it. The radiative transfer equation (RTE) incorporated in the WSGG model is compatible with any general radiation solvers, and free from any restriction.

To take into account the spectral behaviour while retaining the advantage of WSGG idea, Kim and Song [25, 26] proposed a WSGGM-based narrow band (WNB) model. Comparison with the SNB results shows that the error of the WNB model is sufficiently small when examining the radiative heat fluxes over the entire spectrum. To be used in the areas requiring highly accurate spectral properties such as spectral remote sensing techniques [27–28] however, the current spectral error of the WNB model has to be reduced significantly.

The aim of this paper is to modify the WNB model and to demonstrate the possibility of its utilisation in such areas as spectral scanning inversion problems to measure the temperature/concentration profile along a line of sight. For this purpose, the 4.3 μm band of CO_2 is selected because it is a strong infrared band with only a small overlap with a much weaker CO band. In addition, CO_2 is an important combustion product of hydrocarbon fuels and thus it is present in most engineering systems of interest.

In the following section, the WNB model of Kim and Song [26] is briefly described and applied to the 4.3 μm band of CO_2 without any modification. The results are compared with LBL and SNB calculations. The generation of CO_2 spectroscopic database suitable for high temperature is also explained, from which the LBL calculations are obtained as the reference data. It will be shown that the WNB model is suitable elsewhere. Unfortunately however, it is not a good model for the CO_2 4.3 μm band, and further improvement is still to be sought. The modification using the CK concept is explained in § 3, and we examine whether the modification produces good agreement with the LBL calculations. In § 4, the WNB model is further extended with a CKFG concept and the accuracy is also examined. Recommendation of the models is made considering the accuracy and computational efficiency.

2. TEST OF WNB MODEL OF KIM & SONG

Kim and Song [26] proposed a WSGGM-based narrow band model, in which the narrow band-averaged emisssivity is expressed as:

$$\varepsilon_{\mathrm{m}} = \sum_{j=1}^{M} (1 - \mathrm{e}^{-\kappa_j L}) W_j \tag{1}$$

where M is the number of gray gases considered in the modelling. The spectral emissivity ε_{m}, a term used here for narrow band-averaged or low-resolution spectral emissivity, is the weighted sum of the spectral emissivity of gray gases. Among various forms of dependence on temperature and/or pressure, the following type is recommended as being the most accurate:

$$\kappa_j = \kappa_{i0} \frac{P}{T^2} \mathrm{e}^{-\alpha_k / T} (1 - \mathrm{e}^{-hc\eta/kT}) \tag{2}$$

where j stands for a combination of i and k. When there are 8 κ_{i0}'s and 3 α_k's, for instance, then M is 24. This model takes into account the spectral behaviour by applying common model parameters κ_{i0} and α_k to all narrow bands. In addition, this model incorporates the RTE in the absence of scattering as follows:

$$\frac{\mathrm{d}I_j}{\mathrm{d}s} = \kappa_j (W_j I_{\mathrm{b}\eta} - I_j) \tag{3}$$

The intensity I_j, the absorption coefficient κ_j, and the weight W_j correspond to the j'th gray gas. The spectral blackbody intensity $I_{\mathrm{b}\eta}$ within the narrow band may be treated as a constant, as given by the Planck's law,

$$I_{\mathrm{b}\eta} = \frac{2 C_1 \eta^3}{\exp(\eta C_2 / T) - 1} \tag{4}$$

where the constant C_1 is $0.59544 \cdot 10^{-8}$ W·m^{-2}, and the constant C_2 is 1.4388 cm·K. The narrow band interval is taken as 25 cm^{-1} and the wavenumber η is taken at the band centre.

Minimisation of the following modelling error is performed to obtain the optimal model parameters:

$$E = \sum_{T} \sum_{L} \left(\frac{\varepsilon_{\mathrm{t}}}{\varepsilon_{\mathrm{m}}} + \frac{\varepsilon_{\mathrm{m}}}{\varepsilon_{\mathrm{t}}} - 2 \right) \tag{5}$$

Here too the conjugate gradient method is used as the minimisation technique as used by Kim and Song [26]. Model parameters κ_{i0} and α_k as well as the weighting factor W_j have to be optimised in the minimisation procedure of equation (5). A test computation is carried out here from $\eta = 2\,050$ cm^{-1} to $\eta = 2\,450$ cm^{-1} for pure CO_2 having three α_k's, eight κ_{i0}'s, and thus twenty-four W_j's as the optimisation parameters. The temperature and path length ranges considered in the optimisation are 500–2500 K and 0.01–10.0 m, respectively.

In this case, the true spectral emissivity ε_{t} is calculated from an approximate CO_2 spectroscopic database suitable for high temperature as well as for low temperature. This database has been generated by following the approach proposed by Scutaru and et al. [29], in which the 'pragmatic' expressions are used to calculate the required hot band intensities from available

data of similar colder band in HITRAN [2, 30]. The molecular constants associated with the involved levels are computed using the data and method of Chedin [31]. All data available in the level and band tabulation [30] of the 1992 edition of the HITRAN database have been retained. The line positions, intensities, and the vibration-rotation energies of the lower levels involved in the transitions are computed using the formulae of Rothman et al. [30]. Lorentz line shapes are modified by adopting a correction factor [32] dependent on the frequency and temperature. The LBL calculation is carried out at every 0.03 cm^{-1} interval, as the results determined after even finer intervals are found to be almost the same.

Comparison between ε_t and ε_m is made for all narrow bands from 2 050 cm^{-1} to 2 450 cm^{-1}. Relatively poor agreement of the modelled emissivity with the LBL calculation is obtained for overall narrow bands. The worst case is shown in *figure 1* for $\eta = 2\,100$ cm^{-1}. Here and in the following sections, 2 100 cm^{-1} is chosen as the calibration band-centre because this wavenumber shows typical characteristics of low-frequency wing (2 050 to 2 175 cm^{-1}). From this computation, it is anticipated that the current WNB model may produce an unacceptable error in cases where very accurate information for the spectral behaviour is required. As shown in *figure 1*, there are relatively large errors under two conditions: medium path length at high temperature, and long path length at low temperature.

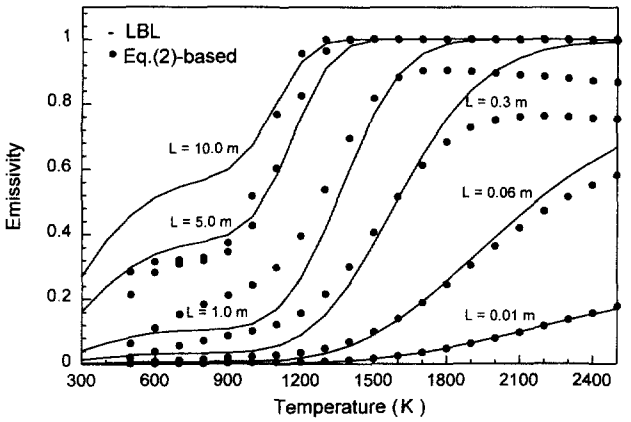

Figure 1. Narrow band emissivity calculations with equation (2)-based WNB model for various temperatures and path lengths at 2 100 cm^{-1}.

Figure 2 shows the spectral normal intensities from 1 m thick layers with parabolic and boundary layer type temperature profiles of reference [26]. The temperature is 1 110 K at the centre and 400 K at both walls in the parabolic profile. The temperature is 300 K at $s = 0$ and 1 500 K at $s = 1.0$ m in the boundary layer profile. The medium is filled with 100 % CO_2 concentration at

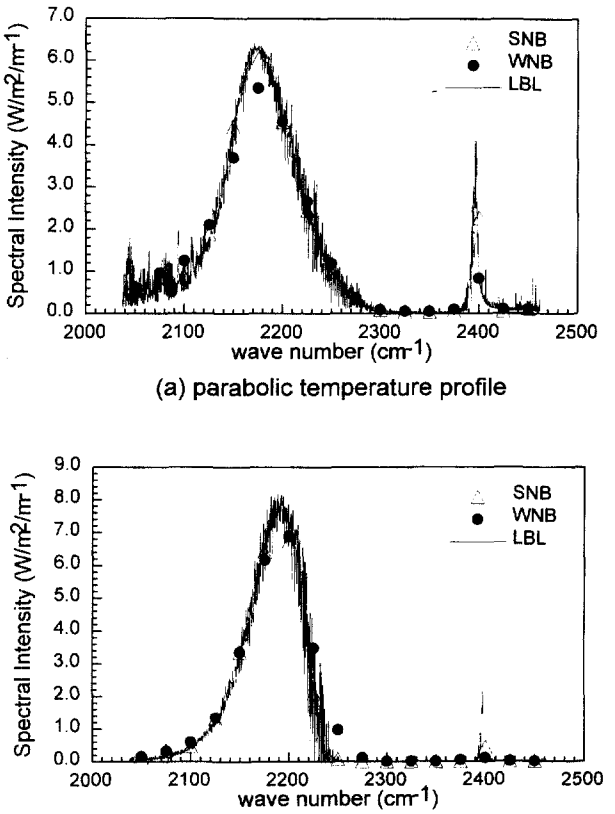

Figure 2. Spectral intensity calculation with equation (2)-based WNB model. (a) Parabolic temperature profile. (b) Boundary layer temperature profile.

1 atm. The following formula is used to compute the wall intensity:

$$I(0) = \sum_{j=1}^{24} \int_0^L \left[W_j \kappa_j(s) I_{b\eta}(s) \exp\left(-\int_0^s \kappa_j(s') \mathrm{d}s' \right) \right] \mathrm{d}s \tag{6}$$

Table I shows the spectral error of various calculations (the CK-based and the CKFG-based computations will be described later) for the two temperature profiles. The quantitative error of the current WNB model is 10 to 20 % except for a few bands for the parabolic temperature profile. For boundary layer profile, the errors between 2 125 cm^{-1} and 2 200 cm^{-1} are acceptable, but the errors at other highly transparent bands are tremendously large. Generally, SNB results are in better agreement though they may not be satisfactory for use in inverse radiative problems. This comparison indicates that the error is too great for the current WNB model to be used for accurate spectral prediction.

TABLE I
Spectral error of intensity calculation referenced to LBL calculation.
(a) parabolic temperature profile.

Band Centre (cm^{-1})	SNB (%)	Equation (2)-based (%)	CK-based (%)	CKFG-based (%)
2 050	14.92	13.97	0.17	0.53
2 075	7.77	29.26	0.16	3.92
2 100	2.97	40.21	2.88	1.41
2 125	2.25	12.94	1.19	0.63
2 150	2.70	14.11	1.64	4.09
2 175	0.51	12.05	0.71	1.08
2 200	2.49	2.32	0.10	1.02
2 225	3.97	3.79	0.07	2.20
2 250	4.38	14.68	0.48	2.85
2 275	3.57	11.56	0.27	6.99
2 300	4.29	5.73	0.25	11.99
2 325	9.01	27.34	0.61	0.73
2 350	1.45	15.96	0.36	0.74
2 375	13.73	35.02	1.42	64.47
2 400	121.99	18.14	36.06	73.12
2 425	54.85	22.49	7.90	8.40
2 450	20.71	23.48	5.10	0.88
(b) Boundary layer temperature profile.				
Band Centre (cm^{-1})	SNB (%)	Equation (2)-based (%)	CK-based (%)	CKFG-based (%)
2 050	53.51	87.13	4.18	6.31
2 075	100.99	91.76	6.29	1.70
2 100	4.69	31.16	1.45	1.15
2 125	1.81	3.92	0.26	1.18
2 150	0.77	0.67	0.21	3.74
2 175	0.40	4.37	1.21	3.35
2 200	3.23	1.20	0.15	0.64
2 225	17.36	37.44	2.69	6.69
2 250	16.69	996.86	6.93	22.42
2 275	16.08	4 157.2	1.30	2.59
2 300	0.10	377.86	0.05	0.04
2 325	0.09	597.10	0.05	0.00
2 350	0.06	219.79	0.04	0.00
2 375	0.52	2 662.8	0.07	0.33
2 400	98.53	50.35	75.24	20.60
2 425	36.13	3.43	7.10	8.79
2 450	2.07	6.99	6.14	1.87

3. MODIFIED WNB MODEL USING CORRELATED-K METHOD

Before any modification of the WNB model is made, one should consider why the previous WNB model produces such great errors as in *figures 1* and *2*. Kim and Song [25, 26] proposed various forms, along with equation (2), for dependence on temperature and/or pressure. Their expression is, however, relatively simple, while, in fact, the modelling parameters κ_{i0} and α_k might be better fitted by allowing variation from one narrow band to another. Thus, this may have resulted in the large discrepancies. Other expressions can be found in other models such as the CK or CKFG model, where the absorption coefficients at seven quadrature points are represented as analytical expressions with at least seven or ten parameters [8].

As the CK model hints, the way to modify the WNB model is by adopting more complicated expressions of absorption coefficients to accommodate different patterns of the spectral emissivity variation at a narrow band. In this study, however, only the dependence on temperature is taken into account because the absorption coefficient is more dependent on temperature than pressure. Direct tabulation of absorption coefficient versus temperature is used rather than carrying out the analytical fitting procedure.

An important assumption in the decision to adopt the WSGGM- based idea is considered next in more detail. When the RTE is integrated over wavenumber intervals of a gray gas, application of the Leibnitz rule produces additional terms in equation (3) which account for variation of a gray gas spectral interval from point to point. The correct calculation of them, however, is too complicated. Denison [33] suggests two assumptions, one simply neglecting the additional Leibnitz terms, the other fixing the boundaries of a gray gas in the η vs. κ_η histogram. He also shows that the former produces greater error than the latter. The histogram boundaries are of themselves fixed in a uniform medium, so the Leibnitz terms are deleted without any erroneous assumption. In non-uniform and inhomogeneous medium, however, the following 'correlated' scaling approximation has to be introduced to fix the histogram boundaries:

$$\kappa_\eta(\eta,T,P,Y_s) = \phi(T,P,Y_s)\varphi(\eta) \tag{7}$$

This assumption says, for instance, if κ_η at η_1 is twice that at η_2 at a temperature, this ratio persists at another temperature. This is the correlated state given by equation (7).

In the RTE shown in equation (3), the weighting factor corresponding to the absorption coefficient κ_j of j'th gray gas is expressed in a narrow band $\Delta\eta$ as:

$$W_j = \frac{\sum_i \Delta\eta_{i,j}}{\Delta\eta} \tag{8}$$

where the subscripts i and j denote the i'th histogram segment of the j'th gray gas absorption coefficient. Then, the weighting factor becomes the integrated segment fractions over a narrow band, as shown by equation (8), because the blackbody intensity is indeed constant within a narrow band. When the above scaling approximation is justified, the weighting factor W_j becomes constant against temperature for a narrow band. *Figure 3* shows the actual shape of absorption lines at three different temperatures around 2 100 cm^{-1}. It is, thus, seen that the actual spectrum approximately satisfies the correlation except for the most significant lines near 2 094 cm^{-1}. For the moment, the effect of these uncorrelated lines is not clearly demonstrated. In this attempt however, all narrow bands near 4.3 μm show similar tendency, so the scaling approximation may be used within an acceptable error.

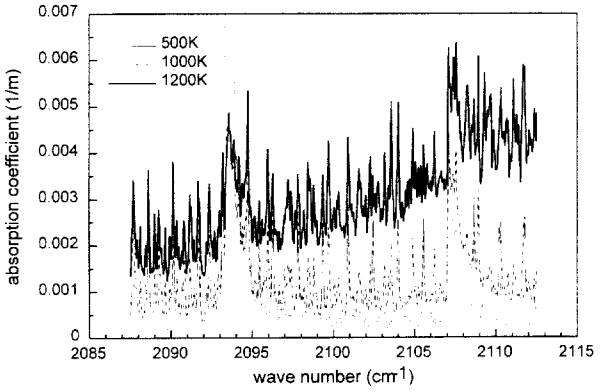

Figure 3. High resolution spectrum of CO_2 at three different temperatures.

It is interesting to compare the definitions of absorption coefficient and weighting factor in the WNB model with those in the CK model. In the CK model, the reordered spectrum is used instead of the actual spectrum, in which the cumulative k-distribution function is defined as:

$$g(T,\kappa) = \frac{1}{\Delta\eta}\int_{\Delta\eta} H(\kappa - \kappa_\eta)\mathrm{d}\eta \qquad (9)$$

The function $H(\kappa - \kappa_\eta)$ is the Heaviside unit function, which is 1 when κ_η is smaller than κ, and 0 otherwise. Since the variations of κ versus g are much smoother than the variations of κ versus η, integrals over g can be calculated using quadratures with a small number of terms. In the CK model, from this definition, the absorption coefficient κ_j is merely a number corresponding to j'th quadrature point and the weighting factor W_j is only a numerical integration factor defined by a quadrature formula. Note, in the WNB model, on the other hand, κ_j is the absorption coefficient of j'th gray gas and W_j is the weighting factor having the physical definition given by equation (8). Although the mathematical and physical interpretations of the CK model and that of the WNB model may be slightly different from each other, the ultimate modelling concept and the method of application are the same for these two models.

The cumulative k-distribution is used to obtain the tabulated absorption coefficients of gray gases under the assumption that the scaling approximation is justified. The following relation is satisfied between the cumulative k-distribution functions of j'th gray gas in two different temperatures, T and T^* :

$$g\ (T,\kappa_j) = g(T^*,\kappa_j^*) \qquad (10)$$

When the value of g function is given at a reference temperature T^* and absorption coefficient κ_j^*, the corresponding absorption coefficient κ_j is obtained implicitly at another temperature T using equation (10). The absorption coefficient κ_j^* at the reference temperature is determined by minimising the error function given as:

$$E = \sum_L \left(\frac{\varepsilon_\mathrm{t}}{\varepsilon_\mathrm{m}} + \frac{\varepsilon_\mathrm{m}}{\varepsilon_\mathrm{t}} - 2\right) \qquad (11)$$

where the path length range is 0.001 to 10.0 m. For the validation of the current CK-based WNB model, seven gray gases are found to be nearly optimal and thus taken. When the number of gray gas is small, an optimisation process is also desirable in the simultaneous determination of κ_j^*'s and weighting factors. After some trials, it is found that the weighting factors may be prescribed more or less arbitrarily but 'properly', and then the κ_j^*'s are numerically optimised when using as many as 7 gray gases. Now that the weighting factors in a narrow band are assigned to all temperatures in common, the set of κ_j's at each temperature is calculated by equation (10). Such sets are tabulated as functions of temperature for later use.

Table II shows the weighting factors used in the computation and the corresponding absorption coefficient obtained at the reference temperature 500 K at band-centre wavenumber 2 100 cm^{-1}. The same values of weighting factors as shown in *table II* are used throughout all narrow bands. The reason why the largest absorption coefficients correspond to a small weighting factors is to represent more precisely the actual spectrum characterised by spikes shown in *figure 3*.

Figure 4 shows almost exact agreement of the spectral emissivity between the CK-based WNB model and the LBL calculation at 2 100 cm^{-1}. Similar excellent agreement is obtained at all narrow bands except at 2 400 cm^{-1} (the higher wavenumber wing). *Figure 5* shows the spectral intensities for the two non-isothermal layers taken previously. The computation results at all narrow bands except at 2 400 cm^{-1} are excellent. As shown in *table I*, for the parabolic temperature profile, the quantitative error of the CK-based WNB model is less than 1 or 2 % except for a few bands at the higher wavenumber wing. For the boundary layer profile, the errors are a little larger at a few bands compared with

TABLE II
Weighting factors and absorption coefficients of 7 gray gases at 2 100 cm^{-1} for CK-based modelling.

	1st	2nd	3rd	4th	5th	6th	7th
weighting factor*	0.045	0.245	0.320	0.245	0.056	0.051	0.038
absorption coeff. (m^{-1})	0.01374	0.04076	0.04719	0.05818	0.2497	0.4048	0.5315

* weighting factors approximated from reference [9].

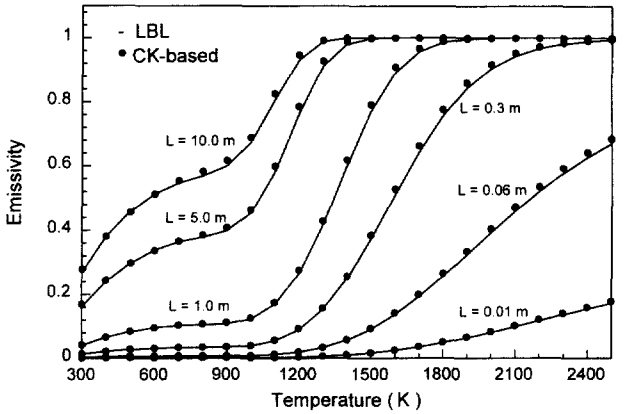

Figure 4. Narrow band emissivity calculations with CK-based WNB model for various temperatures and path lengths at 2 100 cm^{-1}.

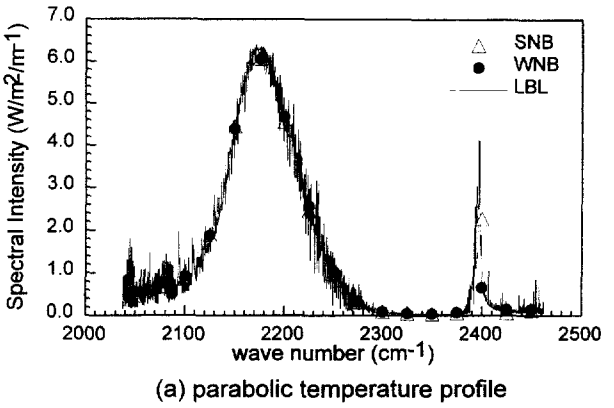

Figure 5. Spectral intensity calculation with CK-based WNB model. (a) Parabolic temperature profile. (b) Boundary layer temperature profile.

the parabolic profile. For both temperature profiles however, the errors are much better than SNB results. The reason why the overall accuracy is significantly improved is not clear, nor why poor agreement is obtained at the higher wavenumber wing. The best guess may be the properness of the assumed model and allowance of variation of κ_j from one narrow band to another. The higher wavenumber wing behaves like an isolated island, as can be observed from *figure 5*. Thus, excluding the higher wavenumber wing, the main band of CO_2 4.3 μm can be very accurately modelled by the current CK-based WNB with about 7 gray gases for future use in inverse radiative problems.

4. FURTHER EXTENSION OF WNB MODEL WITH FICTITIOUS GAS CONCEPT

The computational results in the previous section show that the scaling approximation may be applied to the CO_2 4.3 μm band. A further question arises if the simple scaling approximation is valid under any condition, such as in the case of large temperature gradients for H_2O near the 2.7 μm band. To resolve this case, Rivière et al. [9] proposed the CKFG model, which is an extended CK model with a fictitious gas approach. In the CKFG concept, the real gas is replaced by several fictitious gases to obtain similar variations with temperature. The scaling approximation is assumed to be valid for each fictitious gas, which is characterised by lines corresponding to the same lower level energy E'' of the transition in a given range $\Delta E''$. In short, E'' may be understood as $\alpha_k k/hc$ in equation (2). The spectral lines are sorted according to the values of E'' as are available from the LBL database.

Further extension of the WNB model can also tried with the fictitious gas concept. To derive the RTE in case of three fictitious gases, for instance, equation (3) is modified as:

$$\frac{dI_{i,j,k}}{ds} = \kappa_{i,j,k}(W_{i,j,k}I_{b\eta} - I_{i,j,k}) \qquad (12)$$

where indices i, j and k denote the i'th, j'th and k'th gray gas indices of each fictitious gas. The joint weight $W_{i,j,k}$ is defined as the integrated fraction of the spectral segments overlapped by absorption coefficients of three fictitious gases [34]. The histogram boundaries dividing the spectral overlapped segments is fixed under the condition that each fictitious gas satisfies the scaling approximation. The additional terms appearing due to the Leibnitz rule are thus made to vanish in the RTE. The absorption coefficient corresponding to the joint weight is given as the sum of contributions of the three fictitious gases.

$$\kappa_{i,j,k} = \kappa_i + \kappa_j + \kappa_k \qquad (13)$$

Here κ_i is the absorption coefficient of i'th gray gas in the first fictitious gas, etc. The absorption coefficient of gray gas in each fictitious gas has the same definition as in § 3. The total intensity is then expressed by the following equation (14), as the sum of the solutions shown in equation (12):

$$I = \sum_{i}^{l}\sum_{j}^{m}\sum_{k}^{n} I_{i,j,k} \qquad (14)$$

Here l, m, and n are total number of gray gases in the first, second, and third fictitious gases. The triple summation may produce a significant increase in computational effort because the spectral behaviour of each fictitious gas has to be modelled with a sufficient number of gray gases. When modelling each fictitious gas with seven gray gases, there are in total 343 (7^3) equations to be solved because the total number of solution is the product of the gray gas numbers of each fictitious gas. Therefore, the possibility of reducing the number of gray gases of each fictitious gas without a loss of accuracy has to be investigated.

The spectral range generally contains many lines belonging to absorption band starting from different vibrational levels when fictitious gases are characterised by sufficiently wide $\Delta E''$ for the polyatomic molecules such as H_2O and CO_2. Under these conditions, it can be assumed that fictitious gases have spectra statistically uncorrelated with each other, which makes it possible to express the joint weight as the product of the individual weights, i.e.:

$$W_{i,j,k} = W_i W_j W_k \qquad (15)$$

In this study, the spectral characteristics for each narrow band are modelled with three fictitious gases for each of which three gray gases are taken. Thus, twenty-seven (3^3) solutions are necessary to obtain the total intensity at a given wave number. This number is much larger than the number of gray gases (7) in the previous CK-based WNB model. The fictitious gas are characterised by the lower level energy of the transition as three classes: $E'' < 1\,500$ cm^{-1}, $1\,500$ cm$^{-1} \leqslant E'' \leqslant 3\,000$ cm^{-1}, and $E'' \geqslant 3\,000$ cm^{-1}. Whether the characterised class is suitable or not is reflected in the modelling results. In this paper however, the classification of fictitious gas is chosen by examining the lower energy level of all lines. *Figure 6* shows the actual spectrum of the fictitious gas characterised by $E'' < 1\,500$ cm^{-1} around $2\,100$ cm^{-1}. Other fictitious gas characterised by a different energy level E'' shows similar variations with temperatures. As a result, the dividing criteria in this paper are somewhat arbitrary but fairly reasonable, so that each fictitious gas satisfies almost exactly the scaling approximation.

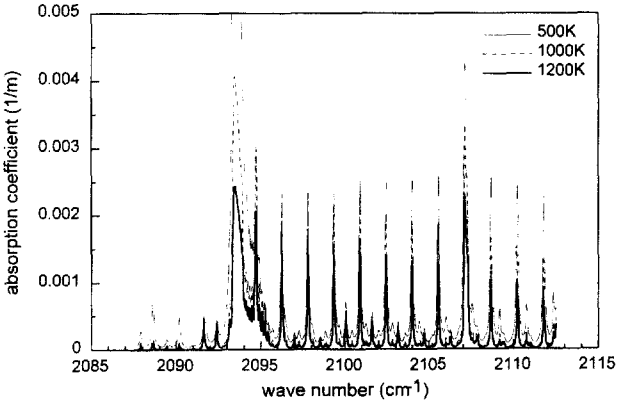

Figure 6. High resolution spectrum of fictitious gas (class 1) for the CKFG-based model at three different temperatures.

The modelling of absorption coefficients and weighting factors in each fictitious gas is carried out using the same method as explained in § 3. The only difference is that weighting factors also become the model parameters in the optimisation procedure because the number of gray gases in each fictitious gas is small, only three. After the absorption coefficients at the reference temperature are determined, the absorption coefficients at other temperatures are obtained by using the cumulative k-distribution, as shown in equation (10), with weighting factors fixed at a narrow band. This process has to be done for every fictitious gases in turn.

Figure 7 shows the cumulative k-distributions of three fictitious gases characterised by the energy level mentioned above for two temperatures, 500 K and 1 000 K. At 500 K, the major contribution in the absorption coefficient of real gas is made by the first and the second fictitious gases. At 1000 K, on the other hand, the major contribution is made by all three fictitious gases. In addition, the absorption coefficient of the first fictitious gas decreases with increasing temperature, as shown in *figure 6*, while those

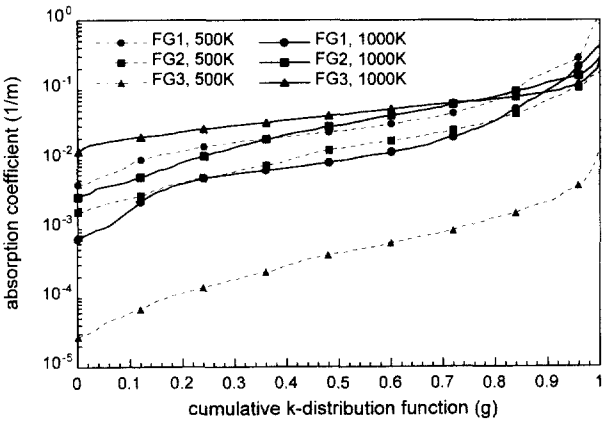

Figure 7. Absorption coefficient vs. $g(\kappa)$ of three fictitious gases for the CKFG-based model at two different temperatures.

of the other two fictitious gases increase with increasing temperature. Especially, the third one consisting of hot lines makes minor contributions at room temperature, but major contributions at higher temperature. This different tendency among three fictitious gases makes the spectral correlation very complex.

After the modelling process in three fictitious gases has been completed, the weighting factors corresponding to the integrated overlapped segments are calculated using equation (15), and the absorption coefficients are tabulated against temperature. *Figure 8* shows the spectral emissivity computed by the extension of the WNB model. Here, the emissivity is given as:

$$\varepsilon_{\mathrm{m}} = \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3}[1 - \mathrm{e}^{-(\kappa_i+\kappa_j+\kappa_k)L}]W_iW_jW_k \qquad (16)$$

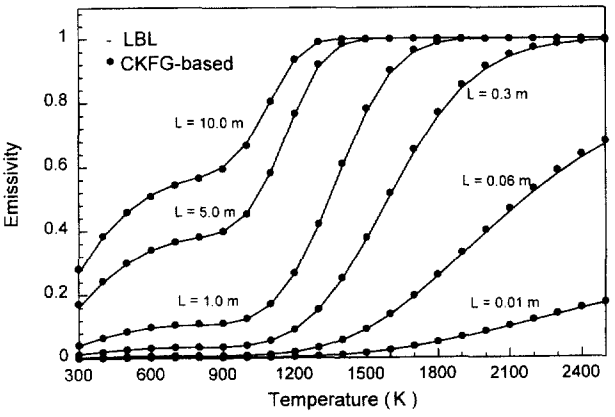

Figure 8. Narrow band emissivity calculations with CKFG-based WNB model for various temperatures and path lengths at 2 100 cm^{-1}.

Very good agreement is also obtained for the CKFG-based WNB model at all narrow bands except at 2 400 cm^{-1}. *Figure 9* shows the spectral intensities for the same non-isothermal layers taken before, which is computed by the following formula:

$$I(0) = \sum_{j=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3} \int_0^L \left[W_iW_jW_k\kappa_{i,j,k}(s)I_{\mathrm{b}\eta}(s)\exp\left(-\int_0^s \kappa_{i,j,k}(s')\mathrm{d}s'\right)\right]\mathrm{d}s \qquad (17)$$

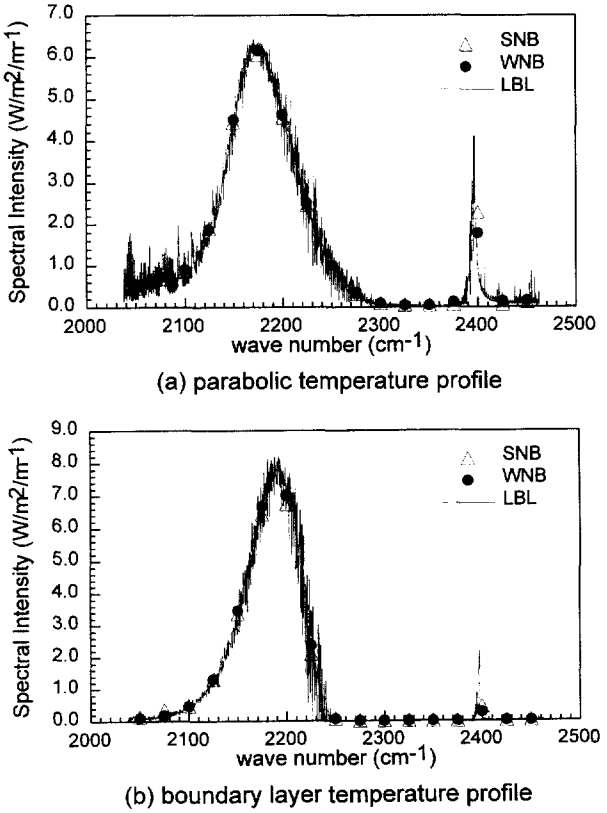

Figure 9. Spectral intensity calculation with CKFG-based WNB model. (a) parabolic temperature profile. (b) boundary layer temperature profile.

The CKFG-based WNB results show excellent agreement with the LBL results. However, according to *table I*, for the parabolic and boundary layer temperature profiles, the quantitative error of the current CKFG-based WNB model is a little larger than that of the previous CK-based WNB model. This is more or less disappointing considering the modelling complexity, increased number of total gray gases (27) and labour. It may indicate that the variation of κ

must be treated with more discretizations than that of the transition energy for the CO_2 4.3 μm band. Nevertheless, this CKFG-based model shows a better or at least equal level of accuracy compared with the SNB results at overall narrow bands.

5. CONCLUSION

This study scrutinises the usefulness of the WNB model in areas requiring highly accurate spectral properties, using the CO_2 4.3 μm band, such as spectral remote sensing techniques. For this purpose, the modelling of the gray gas absorption coefficients is modified from the first simple equation form of Kim and Song, to the second tabulated form based on the cumulative k-distribution function. As the third model, the WNB model is further extended employing the fictitious gas concept to take into account the spectral correlation more precisely. The main issue is whether it is possible to extend the model with an acceptable accuracy without great increase of computational effort.

The first model based on equation (2) results in a greater error and is found to be inappropriate for use in inverse radiative problem. When the WNB model is modified as the CK-based second model with about 7 gray gases, the spectral error may be made small enough to be used in areas requiring highly accurate spectral properties. The third CKFG-based model presented in § 4 shows good agreement with the LBL calculations while the modelling is performed with an increased number (3^3) of gray gases. Among the two new models, however, the CK-based second model exhibits an easier modelling scheme and also better agreement for the CO_2 4.3 μm band. This study will be applied to spectral remote sensing techniques in the future.

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