An accurate efficient and flexible SNBCK-based unified band model for calculations of spectrally resolved and integrated quantities in participating media containing real gases

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An accurate efficient and flexible SNBCK-based unified band model for calculations of spectrally resolved and integrated quantities in participating media containing real-gases

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An accurate, efficient and flexible non-grey gas band model was developed based on the statistical narrow-band model and the correlated-k methodology. Unlike the conventional band models, the new band model provides gas absorption coefficients and can be coupled with any absorption coefficient based solution technique. This band model also offers great flexibility and can be easily tailored to suit different applications such as spectrally resolved quantities or spectrally integrated quantities and different levels of compromise between cpu time and accuracy without reformulation of the model or regeneration of the model parameters. The model can also easily be extended to account for particulate scattering and non-grey surface properties. The accuracy and efficiency of the band model were demonstrated in several examples. The Elsasser narrow-band/Edwards wide-band model was also evaluated against the unified band model.

1. Introduction

Radiative heat transfer plays an important role in many large-scale combustion systems such as furnaces and engines and fire spread in large enclosures. It is also a critical heat loss mechanism in many fundamental flame phenomena in laboratory-scale laminar flames including radiative extinction at small stretch, bifurcation of near-limit premixed flames, and flame-balls. While in many practical applications only the total radiation heat transfer (spectrally integrated) quantities need to be calculated, prediction of spectrally resolved radiation intensities are necessary in some applications such as determining the infrared signature from a rocket exhaust and for remote sensing.

Accurate calculation of radiation heat transfer in flames and combustion systems is quite challenging since it requires adequate treatment of the highly wavelength dependent radiative properties of real-gases (namely CO, CO_2, and H_2O). It has been well established that the grey gas model, though computationally efficient, is in general inaccurate and should not be used in situations where gas radiation is dominant. On the other hand, the ultimate line-by-line (LBL) approach for solving non-grey gas radiation problems is infeasible for calculating practical problems. Various approximate models have also been developed. These include weighted-sum-of-grey-gases (WSGG) models, the exponential wide-band (EWB) model, the statistical narrow-band (SNB) model, correlated-k (CK) and its variant methods, and various hybrid methods that combine a band model and the CK method. The WSGG models offer good computational efficiency but suffer the disadvantages of loss of spectral information and relatively poor accuracy. The conventional wide-band and narrow-band models are not compatible with absorption coefficient based RTE solvers including the popular and accurate discrete-ordinates method (DOM) and are not applicable to scattering problems. The EWB model is less accurate than the SNB model and does not offer adequate spectral resolution for certain applications. Results of the SNB model have often used as benchmark solutions in the absence of LBL results.

The hybrid SNBCK method was first proposed by Lacis and Oinas (1991) for atmospheric applications. Applications of the hybrid SNBCK method to radiative heat transfer problems have been recently made by Liu et al. (1999a and 1999b), Goutière et al. (2000), and Dembele and Wen (2000). This method overcomes the disadvantages of the conventional SNB model, maintains the accuracy of the SNB model and offers much better computational efficiency than the SNB model. However, the original SNBCK method still requires intensive computing time in three-dimensional calculations, especially in gas mixtures due to the band overlapping problem (Goutière et al., 2000). Further improvement in the computational efficiency of the SNBCK method has been recently made by Liu et al. (2000a, 2000b, 2001). In this paper we present a unified band model (UBM) whose bandwidth can be easily switched from a narrow-band (width 25 cm^{-1}) to a wide-band (bandwidth up to 500 cm^{-1}) so that the very same model can be used in different applications. In addition, it can be easily tailored to meet different levels of compromise between cpu time and accuracy without revision of the algorithms.

Due to its simplicity, the spectral absorption coefficient formulation based on the Elsasser narrow-band coupled with the correlation parameters of Edwards' EWB model has gained some popularity in recent years for calculating radiation heat transfer in real-gases (Tong and Skocypec, 1992; Guo and Maruyama, 2000). As the accuracy of this model has not been evaluated against a more accurate model, it was also employed in the present calculations to compare it to the SNBCK method and the UBM.

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2. Formulation

The SNBCK method has been described in previously by Lacis and Oinas (1991) and recently by Liu et al. (2000a, 2001). Therefore the discussion of the SNBCK method itself is kept brief with emphasis given on how the UBM is formed.

The basis of the CK method is that for any spectral radiative quantity φ_ν that is solely dependent on gas absorption coefficient (which is true at a narrow-band where the blackbody intensity function and radiative properties of particulate can be treated as constant) the integration over wavenumber can be replaced by integration over the absorption coefficient, i.e.

$$\overline{\varphi}_\nu = \frac{1}{\Delta\nu}\int_{\Delta\nu}\varphi(\kappa_\nu)d\nu = \int_0^\infty f(k)\varphi(k)dk \tag{1}$$

where $f(k) = 1/\Delta\nu\, d\nu/dk$ is the normalized distribution function of the gas absorption coefficient inside a narrow-band. It is important to realize that when the integration over wavenumber is replaced by integration over the gas absorption coefficient the spectral absorption coefficient κ_ν is replaced by k since it now plays the role of an independent variable and is no longer a function of wavenumber. Application of Eq.(1) to gas transmissivity leads to the conclusion that $f(k)$ is the inverse Laplace transformation of the narrow-band gas transmissivity and provides the theoretical basis to link the SNB model to the CK method. The analytical expression for $f(k)$ corresponding to the SNB gas transmissivity exists and is written as (Lacis and Oinas, 1991)

$$f(k) = \frac{1}{2}k^{-3/2}(BS)^{1/2}\exp\left[\frac{\pi B}{4}\left(2-\frac{S}{k}-\frac{k}{S}\right)\right] \tag{2}$$

The cumulative distribution function $g(k)$, defined as $\int_0^k f(k')dk'$, has also been derived by Lacis and Oinas (1991)

$$g(k) = \frac{1}{2}\left[1-\mathrm{erf}\left(\frac{a}{\sqrt{k}}-b\sqrt{k}\right)\right]+\frac{1}{2}\left[1-\mathrm{erf}\left(\frac{a}{\sqrt{k}}+b\sqrt{k}\right)\right]e^{\pi B} \tag{3}$$

where $a=\frac{1}{2}\sqrt{\pi BS}$, $b=\frac{1}{2}\sqrt{\pi B/S}$ and $\mathrm{erf}(x)$ is the error function. Using the cumulative distribution function, the narrow-band averaged intensity can now be calculated as

$$\overline{I}_\nu = \int_0^1 I(g)dg = \sum_{i=1}^{N} w_i I(g_i) \tag{4}$$

The second half of Eq.(4) is the result of applying a Gauss type numerical quadrature of order N. At a given Gauss quadrature point, the value of the cumulative function g_i is known, the corresponding value of the gas absorption coefficient k_i is then obtained by inverting Eq.(3). Unfortunately an analytical expression for $k = k^{-1}(g)$ does not exist and the value of k for a given value of g has to be found iteratively. Once the gas absorption coefficient k_i is known, a RTE solver is called to calculate the radiation intensity field $I(k_i)$, which is written as $I(g_i)$ in Eq.(4).

The above description of the SNBCK method is applicable only at a non-overlapping narrow-band. When the SNBCK method is used to calculate radiation intensity field in a medium containing more than one radiating gas, the problem of overlapping bands is encountered. Various treatments of overlapping bands have been numerically investigated by Liu et al. (2001). The approximate Malkmus band method described by Liu et al. (2001) was employed in the formulation of the UBM.

When performing numerical calculations using the SNBCK method, the inversion of Eq.(3) consumes a substantial portion of the total cpu time (Liu et al., 2000b). Numerical experiments indicate that a relative error tolerance of 1.0×10^{-2} for the iterative calculation of k_i using Eq.(3) represents a good compromise between computing time and accuracy. The inversion of Eq.(3) was conducted using a Newton-Raphson iteration method with the initial value set to f_{max}. Our numerical experience indicated that the Newton-Raphson method is in general rapidly convergent. However, this iteration method can experience severe difficulties with convergence under certain thermal conditions and at certain Gauss quadrature points when either the derivative dg/dk is very small or the method enters a nonconvergent cycle (Press et al., 1986). In this situation, the bisection method (Press et al., 1986) was used to invert Eq.(3). Therefore, a combined Newton-Raphson and bisection method was employed in the present work.

The SNBCK method discussed above can be used with any RTE solver. The method can be therefore extended to include scattering and non-gray surface properties in a straightforward fashion. The SNB model parameters compiled by Soufiani and Taine (1997) were employed in this work.

Formulation of a UBM based on the SNBCK method is made possible by the observation that the

gas transmissivity over a wide spectral band containing M successive uniform narrow-bands is related to the gas transmissivity over these narrow-bands (Liu et al., 2000b)

$$\bar{\tau}_{WB} = \frac{1}{\Delta\nu_{WB}} \int_{\Delta\nu_{WB}} \exp(-\kappa_\nu L) d\nu = \frac{\Delta\nu_{NB}}{\Delta\nu_{WB}} \sum_{i=1}^{M} \frac{1}{\Delta\nu_{NB}} \int_{\Delta\nu_{NB}} \exp(-\kappa_\nu L) d\nu = \frac{1}{M} \sum_{i=1}^{M} \bar{\tau}_{NB} \tag{5}$$

Similar linear relationships also exist for the distribution function $f(k)$ and cumulative distribution function $g(k)$

$$f_{WB}(k) = \frac{1}{M} \sum_{i=1}^{M} f_{NB,i}(k), \qquad g_{WB}(k) = \frac{1}{M} \sum_{i=1}^{M} g_{NB,i}(k) \tag{6}$$

When the wide band formed by M successive narrow-bands contains overlapping bands, the method of the approximate Malkmus band model proposed by Liu et al. (2001) was employed to convert the overlapping bands to non-overlapping ones with the parameters calculated using the expressions based on the optically thin limit. Gas absorption coefficients at each wide band containing M narrow-bands can be obtained numerically by inverting Eq.(6), $k = g_{WB}^{-1}(k)$. In this UBM, the value of M is a choice of the user and can be any value between 1 (a narrow-band of 25 cm^{-1}) and 20 (a wide-band of 500 cm^{-1}), depending on the application. However, it should be noted that as the value of M increases, the accuracy of the UBM slightly decreases simply because the Planck blackbody intensity function is no longer constant as the bandwidth increases. Larger values of M than 20 are theoretically permitted in the model but at a significant loss of accuracy. A slightly different way to form a wide band model based on the SNBCK method has been recently proposed by Goutière et al. (2001). The regrouping of narrow-bands to form wide bands was carried out by considering the radiative properties of CO_2. They showed that this regrouping strategy slightly improves the accuracy and efficiency over the uniform regrouping method used earlier by Liu et al. (2000a) in the calculations of spectrally integrated quantities. However, their regrouping method does not offer the flexibility of the uniform regrouping one discussed here.

Effects of the order of Gauss numerical quadrature on the accuracy of the SNBCK method, i.e., $N = 1$, for radiation heat transfer have been investigated by Liu et al. (2000a). They found that the calculated spectrally integrated quantities (heat fluxes and radiative source term) are not very sensitive to the order of the Gauss quadrature N as long as $N \geq 2$. Therefore, the need to use a 10-point Gauss quadrature as in the study of Dembele and Wen (2000), to calculate spectrally integrated quantities is questionable. The cpu time of the SNBCK method depends at least linearly on the order of the Gauss quadrature (Liu et al., 2000a). Thus, a substantial saving of cpu time can be achieved by employing a lower order Gauss quadrature without loss of accuracy in the calculation of spectrally integrated quantities. The order of Gauss quadrature N is also a user input parameter in the UBM and any quadrature scheme over [0,1] can be used. Three Gauss type quadrature schemes, the 2-, 4-, and 7-point quadrature, given in Liu et al. (2000a) were used in the present calculations.

The other non-grey gas model considered in this work is the Elsasser narrow-band model (Goody and Yung, 1989)

$$k_{B,\nu} = \rho \frac{S_c}{\delta} \frac{\sinh(\pi\beta/2)}{\cosh(\pi\beta/2) - \cos\left[2\pi(\nu - \nu_c)/\delta\right]} \tag{7}$$

where S_c/δ is the mean-line-intensity-to-spacing ratio given by Edwards' EWB model (Edwards, 1976) as

$$\frac{S_c}{\delta} = \frac{\alpha}{\omega} \exp\left(-a\left|\nu - \nu_c\right|/\omega\right) \tag{8}$$

The band shape factor a is equal to 1 for an asymmetric band and 2 for a symmetric band. It is worth noting that in this model the value of line spacing δ is not specified. Typical values of δ used in the literature are 1 cm^{-1} (Tang and Brewster, 1994) and $30\omega_b$ cm^{-1} (Tong and Skocypec, 1992). The Elsasser narrow-band model coupled with the EWB model has gained some popularity recently due to its simple expression in terms of the gas absorption coefficient (Tong and Skocypec, 1992; Tang and Brewster, 1994; Guo and Maruyama, 2000). However, a critical evaluation of the accuracy of this non-grey gas model against the results from a more accurate model has not been reported. Parameters of the EWB model were calculated using the expressions given in Edwards (1976) along with the efficient procedure suggested by Lallemant and Weber (1996).

3. Results and Discussions

In the following calculations the total pressure is 1 atm. All calculations were conducted on a SGI Octane 175 MHz workstation.

Spectrally resolved intensities along a-line-of-sight

Narrow-band line-of-sight intensities emitted from three gas columns at $x = L_x$ and along x direction were computed using SNB, SNBCK using the three quadratures, and the Elsasser model. The length of the three gas columns is 0.5 m and the total pressure is at 1 atm. Other thermal conditions are summarized below: Column 1, $X_{CO2} = 0.2$, $X_{H2O} = 0.0$, $T = 1000$ K; Column 2, $X_{CO2} = 0.0$, $X_{H2O} = 0.2$, $T = 1000$ K; Column 3, $X_{CO2} = 0.1$, $X_{H2O} = 0.2$, and a parabolic temperature distribution with 500 K at boundaries and 2000 K at the center. In the calculation using the Elsasser model, each narrow band of 25 cm^{-1} width was further divided into 4 uniform segments. The gas columns were divided into 25 uniform divisions in all the calculations. Narrow-band integrated intensities from Column 1 are compared in Fig.1. Results of the SNBCK7 (using the 7-point quadrature) are in very good agreement with those of the SNB model. The narrow-band intensities are not reproduced well by the Elsasser model. Also shown in Fig.1 are the total (spectrally integrated) intensities from the SNB, the SNBCK with different quadratures, and the Elsasser model. The total intensities from the SNB and SNBCKn (n=2,4,7) differ only slightly. The Elsasser model also predicts a reasonably accurate integrated intensity under these conditions, being only about 4.6% lower than the SNB value. Fig.2 shows the narrow-band integrated intensities from Column 2 obtained using the SNB, SNBCK7, and the Elsasser model. Again the SNBCK7 intensities are in very good agreement with those of the SNB. However, the narrow-band intensities based on the Elsasser model are in serious error. The spectrally integrated intensities based on the SNBCKn (n= 2,4,7) are in excellent agreement with that of the SNB model. The Elsasser model underpredicts the total intensity by about 20%. Results from Column 3 are compared in Fig.3. In this non-isothermal case, there are some discrepancies in the narrow-band intensities between SNBCK7 and SNB, particularly in the spectral region 2300-2400 cm^{-1}. Otherwise, the agreement between the results of these models is very good. The Elsasser model does not capture the detailed spectral distribution of the intensity. As far as the total intensity is concerned, however, the Elsasser model performs reasonably well, with only about 10% lower than the SNB intensity.

Radiative transfer in one-dimensional parallel-plate

The one-dimensional parallel-plate case considered here contains a uniform gas mixture of CO_2, H_2O, and N_2. The separation distance is 5 m. The two boundaries are cold and black. The thermal conditions are the same as those in Column 3 described above. The domain was divided into 101 uniform segments. RTE was solved using DOM along with T_3 quadrature (Thurgood et al., 1995). The cpu time and the wall heat flux from UBM and the Elsasser model with various values of N and M are compared in Table 1. Errors of UBM remain less than 7%. Errors of the Elsasser model are between 12 to 20%. UBM with $N = 4$ and $M = 10$ offers a near order-of-magnitude decrease in cpu time with an error < 3%. Further decreases in cpu time is accompanied by substantial decrease in accuracy.

Radiative transfer in three-dimensional rectangular enclosure

DOM was employed to solve the RTE in cartesian coordinates along with the step spatial differencing scheme and the T_4 angular quadrature (Thurgood et al., 1995). The dimension of the enclosure is $2m(L_x)\times2m(L_y)\times8m(L_z)$. The enclosure is divided into $17\times17\times40$ control volumes. The division in x and y directions is uniform. Non-uniform grids are used in the z direction to better resolve the large temperature gradient region. The walls are black and at 300 K. The mole fraction distributions of CO_2 and H_2O in the enclosure are assumed to be uniform at 0.1 and 0.2, respectively. Non-uniform temperature distribution is specified as $T = (T_{axis} - 800) f(r) + 800$ where T_{axis} and $f(r)$ define the temperature distribution along the centerline and radial direction, respectively, with $T_{axis} = 400 + (2100 - 400)z/0.75$ for $z < 0.75$ m and $T_{axis} = 800 + (2100 - 800)(8 - z)/7.25$ for $z > 0.75$ m. $f(r)$ is given as $f(r) = 1 - 3r^2 + 2r^3$ with r being the distance to the centerline. In the four corner regions where r is greater than 1 m, r simply takes the value of 1 m.

Figure 4 compares the source term distribution along the centerline calculated using UBM and the Elsasser model with various values of N and M. In order to highlight the discrepancies between results of different methods, an enlarged version of Fig.4 around the minimum source term value is presented in Fig.5 along with the cpu times of the two methods. Fig.5 shows that the accuracy of the UBM is insensitive to the value of N but more sensitive to M in this 3D case. This is expected since the blackbody intensity is no longer constant as the band width increases (increasing M). The UBM is consistently more accurate than the Elsasser model, except when using $N = 2$ and $M = 40$ where the errors are similar. Unlike in the 1D parallel-plate case, the cpu time monotonically decreases with increasing M at a given N. This behavior is the result of the relatively small portion of the cpu time required in the inversion of $g(k)$ relative to the cpu time spent on solving the RTE in the 3D

calculations. The cpu times of the UBM with $N = 2$ and $M = 10$ or 20 are comparable to that of the Elsasser model with $N = 2$ and $M = 20$, being within a factor of 2. However, the UBM is more accurate, especially when using $M = 10$. Note that use of $N = 2$ and $M = 10$ and 20 results in respectively 72 and 36 spectral discretisation points. Such a spectral resolution is also comparable to that used by Guo and Maruyama (2000) who divided the spectral range 100 to 10000 cm^{-1} into about 100 sub-bands. Therefore, the UBM is preferred in calculations of radiation heat transfer in real-gases. The net wall heat flux distributions along z at $x = 2$ m and $y = 1$m are shown in Fig.6. Once again, the UBM is more accurate than the Elsasser model.

Table 1. Comparison of cpu time and wall heat flux for the 1D parallel-plate test case.

N	M	Cpu, s	Wall heat flux, kW/m^2
UBM			
7	1, exact	18.8	119.608
7	1	10.6	119.174
7	10	4.9	118.651
7	20	5.3	117.464
4	1	4.8	122.613
4	10	2.0	122.750
4	20	2.2	126.744
2	1	2.4	125.099
2	10	0.98	125.375
2	20	1.1	124.168
Elsasser			
4	1	7.8	105.469
4	10	0.8	100.150
4	20	0.4	95.499

4. Conclusions

A flexible and accurate unified band model was developed in this study. This model can be used in a wide range of applications since it accurately predicts both the spectrally resolved radiation intensity and the spectrally integrated quantities with good efficiency. The unified band model essentially retains the accuracy of the statistical narrow-band model while offers significant improvement in efficiency. In addition, it can be used for problems with radiation scattering and/or non-grey boundaries in a straightforward way. When using $N = 2$ and $M = 10$ or 20, the unified band model is not only more accurate than the Elsasser model, but also offers comparable efficiency for calculations of spectrally integrated quantities. The Elsasser model should not be used in problems where spectrally resolved information is required.

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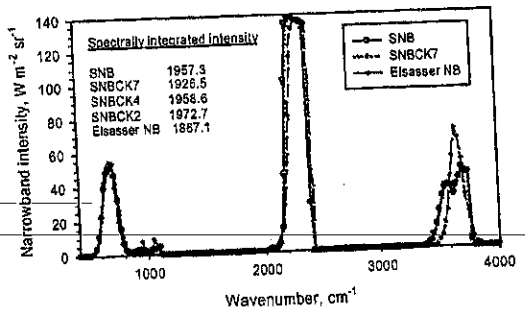

Fig.1 Narrow-band integrated intensities emitted from Column 1 with cpu times (s).

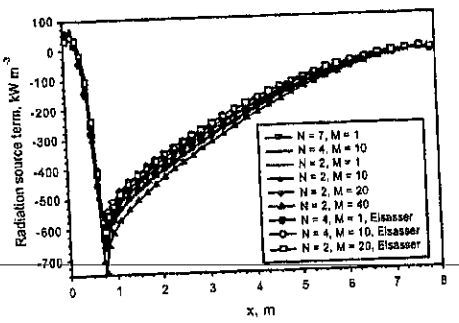

Fig.4 Source term distributions along the centerline of the enclosure using UBM and the Elsasser model.

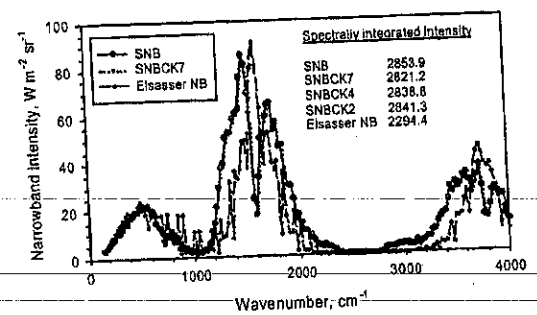

Fig.2. Narrow-band integrated intensities emitted from Column 2 with cpu times (s).

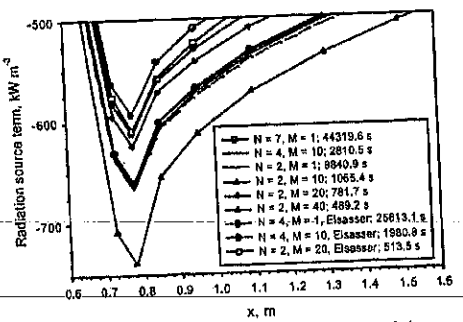

Fig.5 An enlarged version of Fig.4 around the minimum source term with cpu time indicated.

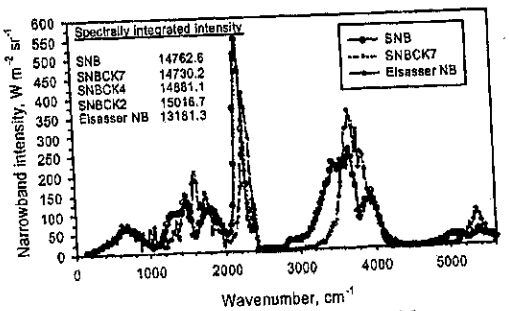

Fig.3 Narrow-band integrated intensities emitted from Column 3 with cpu times (s).

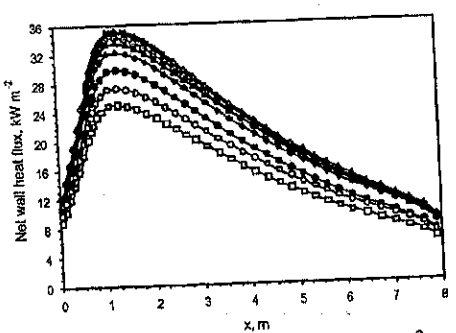

Fig.6 Net wall heat flux distributions along z at $x = 2$ m and $y = 1$ m. See Fig.4 for legend.

Abstract

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