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SCALABLE MULTI-GROUP FULL-SPECTRUM CORRELATED- k DISTRIBUTIONS FOR RADIATIVE TRANSFER CALCULATIONS

Hongmei Zhang and Michael F. Modest
 Mechanical Engineering Department
 The Pennsylvania State University
 University Park, PA16802
 Email: mfm@mara.me.psu.edu

ABSTRACT

A new full-spectrum k -distribution method has been developed, in which spectral locations are sorted into M spectral groups, according to their absorption coefficient dependence on (partial) pressure and temperature. Calculating correlated- k full-spectrum k -distributions for each of the M groups, LBL accuracy can be obtained with $M \leq 32$. Database values have been assembled for CO₂ mixtures at atmospheric pressure. The method is fully scalable, i.e., spectral groups from the database can be combined to obtain coarser group models ($M = 1, 2, 4, \dots$) for greater numerical efficiency (accompanied by slight loss in accuracy).

NOMENCLATURE

a = weight function for FSCK method
 A = parameter in the scaling function
 b = self broadening-to-air broadening coefficient
 b_{self} = self-broadening line half-width, cm⁻¹
 b_{air} = air-broadening line half-width, cm⁻¹
 E = parameter in the scaling function, K
 f = k -distribution function, cm
 g = cumulative k -distribution
 I = radiative intensity, W/m²sr
 k = absorption coefficient variable, cm⁻¹
 k_{η} = spectral absorption coefficient at reference state, cm⁻¹
 l = geometric length, m
 n = scaling function parameter
 p = pressure, bar

q = radiative heat flux, W/m²
 s, s' = distance along path, m
 T = temperature, K
 u = scaling function for absorption coefficient
 w = weight function
 x, \underline{x} = mole fraction (vector)

Greek Symbols

η = wavenumber, cm⁻¹
 ϕ = composition variable vector
 $\bar{\Phi}$ = scattering phase function
 κ = absorption coefficient, cm⁻¹
 Ω = solid angle, sr
 σ_s = scattering coefficient, cm⁻¹

Subscripts

0 = standard state for database
 b = blackbody emission
 j = line or bin
 m = spectral group
 max = maximum
 min = minimum
 P = Planck Mean
 ref = reference condition for problem at hand
 w = wall
 η = spectral

INTRODUCTION

Radiative transfer in absorbing-emitting gas mixtures can be most accurately predicted using the line-by-line approach, but

LBL calculations require large computer resources and computational time. It has been known for some time that, for a narrow spectral range (i.e., a range over which the Planck function $I_{b\eta} \approx \text{const}$) in a homogeneous medium (i.e., absorption coefficient κ_η is not a function of spatial location), the absorption coefficient may be reordered into a monotonic k -distribution, which produces exact results at a tiny fraction of the computational cost [1,2]. As with other narrow band models, treatment of nonhomogeneous media was somewhat problematic. Two methods have been commonly used to address nonhomogeneity: the *scaling approximation* and the assumption of a *correlated k -distribution*. The Correlated- k method has been shown to be accurate primarily for low temperature meteorological applications [1, 3, 4].

More recently, the reordering concept has also been applied to the full spectrum. Denison and Webb [5, 6] developed the Spectral-Line-Based Weighted-Sum-of-Gray-Gases (SLW) model, in which line-by-line databases are used to calculate weight factors for the popular WSGG model [7, 8]; for nonhomogeneous gases they used the correlated- k approach. A similar method, called the Absorption Distribution Function (ADF) approach, was developed by Rivière et al. [9, 10].

Very recently, Modest and Zhang [11] demonstrated how k -distributions can be obtained for the entire spectrum, calling it the FSCK method. Their approach differs from the SLW and ADF approaches in two respects: (1) they obtained a continuous k -distribution, rather than the stepwise WSGG method [showing that the SLW/ADF/WSGG methods are crude step implementations of the full-spectrum k -distribution (FSCK) method]; and (2) they used the scaling approximation, to make a clear mathematical development of the method possible for inhomogeneous media. In addition, they introduced a somewhat more elaborate scheme for establishing a reference state, which further improves accuracy.

These full-spectrum methods can achieve LBL accuracy for homogeneous media, but at a tiny fraction of the computational cost. However, substantial inaccuracies can occur in nonhomogeneous media, because the assumptions of a correlated or scaled absorption coefficient are violated, particularly in the presence of extreme temperature changes and/or changing mole fractions. To overcome this limitation, Pierrot et al. [10] developed the fictitious-gas-based ADF, in which the individual lines comprising the absorption coefficient were placed into separate groups based on their temperature dependence. While improving accuracy, the method becomes calculatingly more expensive by a factor of M^2 , where M is the number of fictitious gases or groups, in order to deal with line overlap from different fictitious gases. Similarly, Zhang and Modest [12] extended their FSCK method to such fictitious gases. Their method, called the (multi-scale) MSFSCK method, increases computer time only by a factor of M , since fictitious-gas overlap is treated in an approximate fashion.

The subtle differences between correlated and scaled absorp-

tion coefficient were recently detailed by Modest [13]: an absorption coefficient attains a value $\kappa_\eta(\eta, \underline{\phi}_{\text{ref}}) = k_{\text{ref}}$ many times across the spectrum, where the composition variables $\underline{\phi} = (T, p, \underline{x})$ are evaluated at a reference condition. If, at every one of these spectral locations, the absorption coefficient at a different state has also a single specific value $\kappa_\eta(\eta, \underline{\phi}) = k(\underline{\phi}, k_{\text{ref}})$, i.e., k may be a function of k_{ref} , but not of η directly, and if k is a monotonically increasing function of k_{ref} , then κ_η is correlated. The absorption coefficient is scaled if this k is independent of k_{ref} . Thus, we may write

$$\text{correlated:} \quad \kappa_\eta(\eta, \underline{\phi}) = \kappa_{\eta, \text{ref}}(\eta, \underline{\phi}_{\text{ref}}) u(\underline{\phi}, \underline{\phi}_{\text{ref}}, \kappa_{\eta, \text{ref}}) \quad (1)$$

$$\text{scaled:} \quad \kappa_\eta(\eta, \underline{\phi}) = \kappa_{\eta, \text{ref}}(\eta, \underline{\phi}_{\text{ref}}) u(\underline{\phi}, \underline{\phi}_{\text{ref}}) \quad (2)$$

It follows that scaling is more restrictive, i.e., a scaled absorption coefficient is always correlated, but not vice versa. The FSCK method of Modest and Zhang [11] can be used with either model, and should then be more properly called FSSK (full-spectrum scaled k -distribution) and FSCK methods.

It is the purpose of the present paper to introduce a new full-spectrum method, in which spectral positions (with absorption coefficients consisting of contributions from many different lines) are placed into spectral groups according to their dependence on temperature and (partial) pressure (as opposed to the ADFFG and MSFSCK methods, which place spectral lines into groups, each of them affecting the absorption coefficient over many different wavenumbers). Such a model avoids the problem of overlap between different groups. In addition, it allows the consideration of partial pressure dependence during the grouping process. Total pressure variations could be incorporated as well, and will be considered in follow-up work.

THEORETICAL DEVELOPMENT

Spectral Grouping

Consider the top frame of Fig. 1, which shows the absorption coefficient of CO_2 for a small part of its $4.3\mu\text{m}$ band, for a temperature of 300 K, and a total pressure of 1 bar, and a mole fraction of 10%. This absorption coefficient contains the contributions from about 1,500 lines (at 300 K). Also shown is the ratio $u = \kappa_\eta(2000\text{ K}, 1\text{ bar}, 10\%) / \kappa_\eta(300\text{ K}, 1\text{ bar}, 10\%)$ (now with contributions from more than 5,000 lines at 2000 K due to the emergence of “hot lines”). Clearly, for such temperature differences, the absorption coefficient is neither scaled ($u = \text{const}$), nor is it correlated [u is a function of $\kappa_\eta(300\text{ K})$ only]. To obtain an absorption coefficient that more closely follows the rules of “scaling” or “correlation,” we may want to break up the spectrum into two groups, throwing all wavenumbers with $u \leq 10$ into “Group 1” and the rest into “Group 2,” as indicated in the bottom frames of Fig. 1. Such simple grouping of the absorption coefficient substantially improves the accuracy of the FSSK and FSCK models,

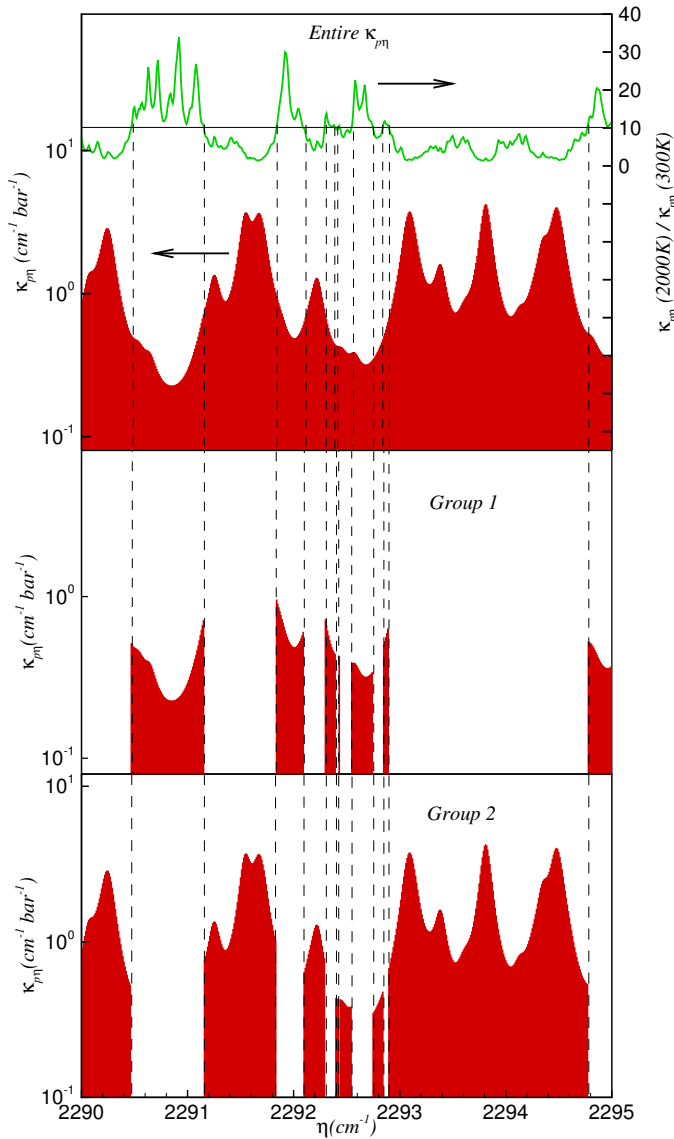


Figure 1. A small portion of the 15 μm CO₂ band is broken up into two groups using Multi-Group approach.

although reaching LBL accuracy will require more sophisticated grouping. This is demonstrated in Fig. 2, which depicts nondimensional heat loss from the cold end of a two-temperature mixture of 10% CO₂-90% air. The slab consists of a $l_h = 50$ cm hot layer at $T_h = 2000$ K, and a cold layer at 300 K of varying width l_c ; both sides are bounded by cold, black walls. The figure shows that, without grouping, the FSK method makes a maximum error of 10.3% for a large cold layer. The FSSK method considerably outperforms the FSK results with a maximum error of 4.4%. The reason is that, without grouping, the assumption of a correlated k -distribution is a bad one in the pres-

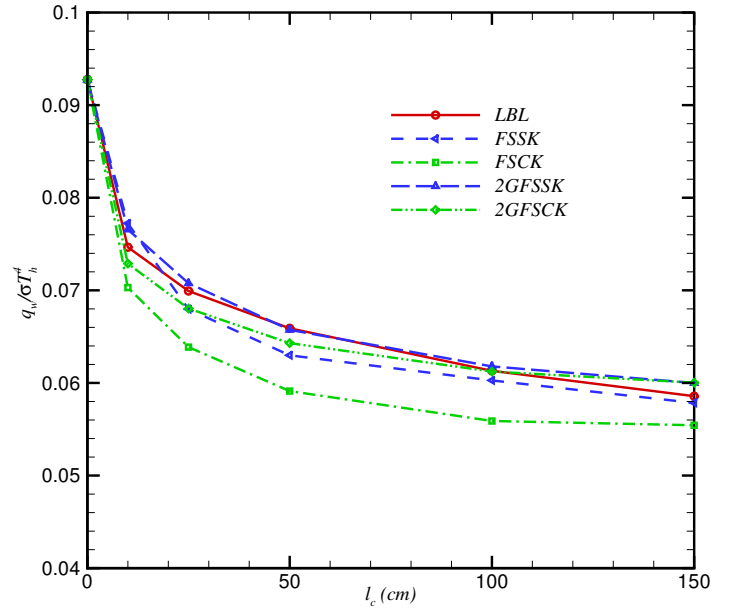


Figure 2. Two-Group results for the heat flux exiting from the cold column of a two-column CO₂-nitrogen mixture at different temperatures ($T_{\text{hot}} = 2000\text{K}$, $l_{\text{hot}} = 50\text{cm}$; $T_{\text{cold}} = 300\text{K}$, l_{cold} variable; uniform $p = 1\text{bar}$, $x_{\text{CO}_2} = 0.1$, cold and black bounding walls).

ence of such large temperature differences, while the u -function can be optimized for this problem in the FSSK method [13]. The simple two-group model indicated in Fig. 1 results in substantial improvement, reducing the maximum error to about 2.5%. It is interesting to note the 2GFSSK and 2GFSSK models perform about equally well: apparently, simply separating absorption coefficients governed by hot lines from those present at low temperature, results in a fairly well correlated distribution.

To achieve accuracies close to those of line-by-line calculations for arbitrary, nonhomogeneous fields, a wide range of temperatures needs to be considered, and a large number of spectral groups needs to be established (variations with mole fractions tend to be much weaker, especially for CO₂, and will be treated as a secondary effect.)

The Multi-Group FSK Approach

The multi-group versions of the FSSK and FSK methods can essentially be developed in the same way as the underlying single group models that were developed by Modest and Zhang [11]. Consider the spectral radiative transfer equation (RTE) for an absorbing, emitting and scattering medium [14]

$$\frac{dI_\eta}{ds} = \kappa_\eta(\underline{\phi}, \eta) [I_{b\eta}(T) - I_\eta] - \sigma_s \left[I_\eta - \frac{1}{4\pi} \int_{4\pi} I_\eta(\hat{s}') \Phi(\hat{s}, \hat{s}') d\Omega' \right], \quad (3)$$

subject to the restriction that scattering properties σ_s and Φ (as well as bounding wall reflectance) are gray. The RTE is now multiplied by the Dirac-delta function $\delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta))$, and integrated across the m -th spectral group $[\eta_m]$ (containing all the wavenumbers for that group). Assuming the absorption coefficient for the m -th group to be correlated, this leads to

$$\frac{dI_{km}}{ds} = k(\underline{\phi}, k_m) \left[f_m(T, \underline{\phi}_{\text{ref}}, k_m) I_b(T) - I_{km} \right] - \sigma_s \left[I_{km} - \frac{1}{4\pi} \int_{4\pi} I_{km}(\hat{s}') \Phi(\hat{s}, \hat{s}') d\Omega' \right], \quad (4)$$

where

$$I_{km} = \int_{\eta \in [\eta_m]} I_\eta \delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)) d\eta \quad (5)$$

$$f_m(T, \underline{\phi}_{\text{ref}}, k_m) = \frac{1}{I_b(T)} \int_{\eta \in [\eta_m]} I_{b\eta}(T) \delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)) d\eta, \quad (6)$$

is the full-spectrum k -distribution for the m -th group, which depends on local temperature through the Planck function, and a reference state $\underline{\phi}_{\text{ref}}$ through the choice of state for $\kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)$. The first term on the right-hand-side of equation (4) uses the assumption of a correlated absorption coefficient, since the absorption coefficient can only be removed from the integral

$$\int_{\eta \in [\eta_m]} \kappa_\eta(\underline{\phi}, \eta) I_{b\eta}(T) \delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)) d\eta = k(\underline{\phi}, k_m) \int_{\eta \in [\eta_m]} I_{b\eta}(T) \delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)) d\eta, \quad (7)$$

if $\kappa_\eta(\underline{\phi}, \eta)$ attains identical values for each wavenumber, where $\kappa_\eta(\underline{\phi}, \eta) = k_m$. As for the single group model, the development is completed by replacing the inconvenient k_m -variable (which leaves the ill-behaved k -distribution f_m in the RTE) by the cumulative k -distribution evaluated at a reference temperature T_{ref} ,

$$g_m(T_{\text{ref}}, \underline{\phi}_{\text{ref}}, k_m) = \int_0^{k_m} f_m(T_{\text{ref}}, \underline{\phi}_{\text{ref}}, k_m) dk_m. \quad (8)$$

This is achieved by dividing equation (4) by $f_m(T_{\text{ref}}, \underline{\phi}_{\text{ref}}, k_m)$, leading to

$$\frac{dI_{gm}}{ds} = k_m(T_{\text{ref}}, \underline{\phi}, g_m) \left[a_m(T, T_{\text{ref}}, g_m) I_b(T) - I_{gm} \right] - \sigma_s \left[I_{gm} - \frac{1}{4\pi} \int_{4\pi} I_{gm}(\hat{s}') \Phi(\hat{s}, \hat{s}') d\Omega' \right], \quad (9)$$

with

$$I_{gm} = \int_{\eta \in [\eta_m]} I_{b\eta}(T) \delta(k_m - \kappa_\eta(\underline{\phi}_{\text{ref}}, \eta)) d\eta / f_m(T_{\text{ref}}, \underline{\phi}_{\text{ref}}, k_m), \quad (10)$$

$$a_m(T, T_{\text{ref}}, g_m) = \frac{f_m(T, \underline{\phi}_{\text{ref}}, k_m)}{f_m(T_{\text{ref}}, \underline{\phi}_{\text{ref}}, k_m)}. \quad (11)$$

While f_m varies over many orders of magnitude with thousands of maxima and minima, the weight function $a_m(T, T_{\text{ref}}, g_m)$ is much better behaved [11], facilitating integration. Note that the correlated $k(\underline{\phi}, k_m)$ was rewritten as [13]

$$k(\underline{\phi}, k_m) = k(T_{\text{ref}}, \underline{\phi}, g_m), \quad (12)$$

where $k(T_{\text{ref}}, \underline{\phi}, g_m)$ is the inverse of

$$g_m(T_{\text{ref}}, \underline{\phi}, k_m) = \int_0^{k_m} f_m(T_{\text{ref}}, \underline{\phi}, k_m) dk_m. \quad (13)$$

This is a consequence of the assumption of correlated k -distributions, postulating that $f_m(T, \underline{\phi}, k_m)$ and $f_m(T, \underline{\phi}_{\text{ref}}, k_m)$ have identical cumulative k -distributions g_m (for any Planck function temperature). Therefore, evaluation of I_{gm} requires the precalculation of two sets of full-spectrum k -distributions for each of the M spectral groups: (i) k -distributions $f_m(T, \underline{\phi}_{\text{ref}}, k_m)$, evaluated for the absorption coefficient taken at reference conditions and for all Planck function temperatures (for the determination of a_m), and (ii) k -distributions $f_m(T_{\text{ref}}, \underline{\phi}, k_m)$, with the absorption coefficient evaluated at local conditions, but the Planck function only at the reference temperature [for the evaluation of $k(T_{\text{ref}}, \underline{\phi}, g_m)$]. Once I_{gm} has been found using any arbitrary RTE solution method, total intensity is determined by summing over all spectral groups and integrating over g -space, i.e.,

$$I = \int_0^\infty I_\eta d\eta = \sum_{m=1}^M \int_0^1 I_{gm} dg. \quad (14)$$

Note that the reference state $\underline{\phi}_{\text{ref}}$ is the only state where the absorption coefficient is taken in its exact form and that a correlated absorption coefficient is assumed for all other states. Therefore, it is important to choose an optimal reference state for each problem at hand. While any arbitrary value can be used for the reference Planck function temperature, it is usually set to the same value as the temperature for the reference state $\underline{\phi}_{\text{ref}}$.

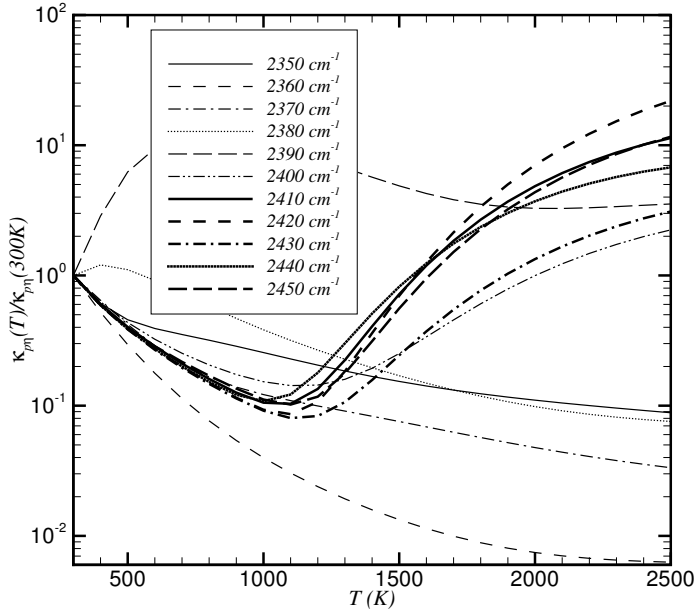


Figure 3. The scaling function u_η for several spectral locations across the 2350-2450 cm^{-1} spectral range of CO_2 .

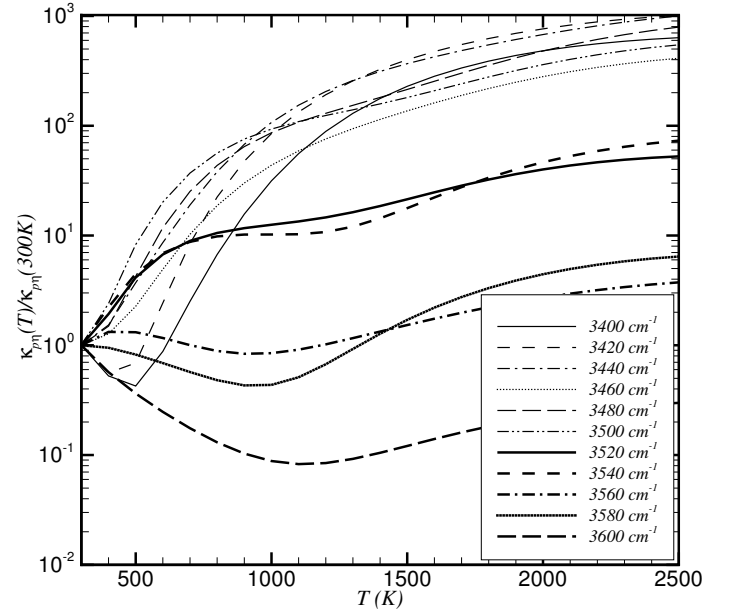


Figure 4. The scaling function u_η for several spectral locations across the 3400-3500 cm^{-1} spectral range of CO_2 .

Databasing of Spectral Groups

To aid with the grouping of spectral location it is of advantage to observe the typical behavior of the scaling function

$$u_\eta(\underline{\phi}, \underline{\phi}_0, \eta) = \frac{\kappa_\eta(\underline{\phi}, \eta)}{\kappa_\eta(\underline{\phi}_0, \eta)}, \quad (15)$$

as it varies across the spectrum, where $\underline{\phi}_0$ is any arbitrary standard state to be compared with (and is not related to the reference state of the previous section). Some typical results are shown in Figs. 3 and 4 for a mixture containing 10% CO_2 , for a few selected spectral locations across the 2350-2450 cm^{-1} (4.3 μm band) and 3400-3500 cm^{-1} (2.7 μm band) ranges. This behavior is seen to be consistent for all spectral locations, and also consistent with theoretical predictions for the absorption coefficient: for a spectral location dominated by cold lines at 300 K, the scaling function first decreases as predicted from the temperature dependence of the rotational and vibrational partition function and of line widths. At some elevated temperature “hot lines” with large lower-level energies wake up, causing a strong increase in u . Based on a thorough investigation of CO_2 scaling function

behavior, a set of 32 scaling functions were chosen as

$$u_m(T, x; T_0, x_0) = \frac{1 + bx \sqrt{\frac{T_0}{T}} + A_m \left[1 + bx \left(\frac{T_0}{T} \right)^2 \right] e^{-E_m/T}}{1 + bx_0 \sqrt{\frac{T_0}{T}} + A_m \left[1 + bx_0 \left(\frac{T_0}{T} \right)^2 \right] e^{-E_m/T_0}} \left(\frac{T_0}{T} \right)^{n_m}, \quad (16)$$

and are shown in Fig. 5 (here arbitrarily normalized with $T_0 = 300\text{K}$ and $x_0 = 0.1$ for better discernibility). Each of the scaling functions is defined by the three parameters A_m , E_m and n_m , and a self broadening-to-air broadening coefficient defined as

$$b = \frac{b_{\text{self}}}{b_{\text{air}}} - 1, \quad (17)$$

where b_{self} is line width due to self broadening, and b_{air} the one due to air broadening. This ratio is fairly constant across the entire spectrum for all gases. For CO_2 , it is approximately 0.3, which was chosen for all 32 groups here. With the group of scaling functions defined, a scan is made across the entire spectrum (in steps of $\Delta\eta = 0.01 \text{ cm}^{-1}$), evaluating the absorption coefficient from the HITEMP database [15] at a standard mole fraction of $x_0 = 0.1$, for a large set of J temperatures $300 \text{ K} \leq T_j \leq 2500 \text{ K}$. The spectral group into which wavenumber η_i is placed, $m(\eta_i)$, is found from minimization, i.e., by finding the group m , which

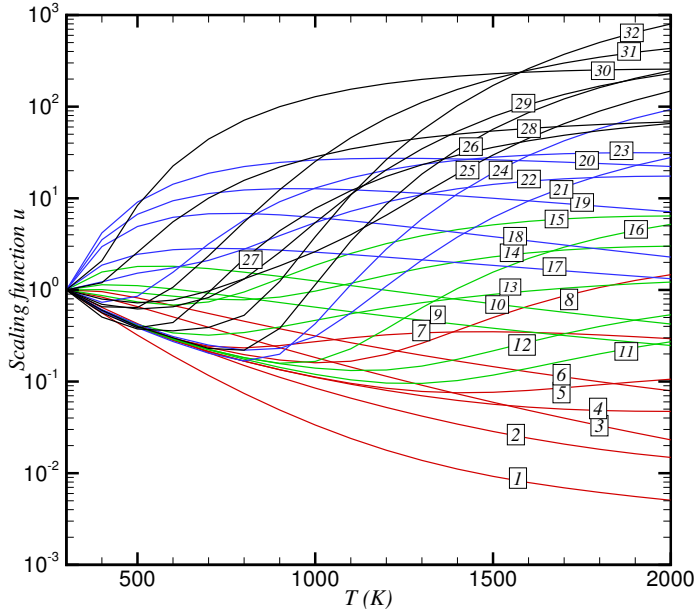


Figure 5. Standard scaling functions for CO₂.

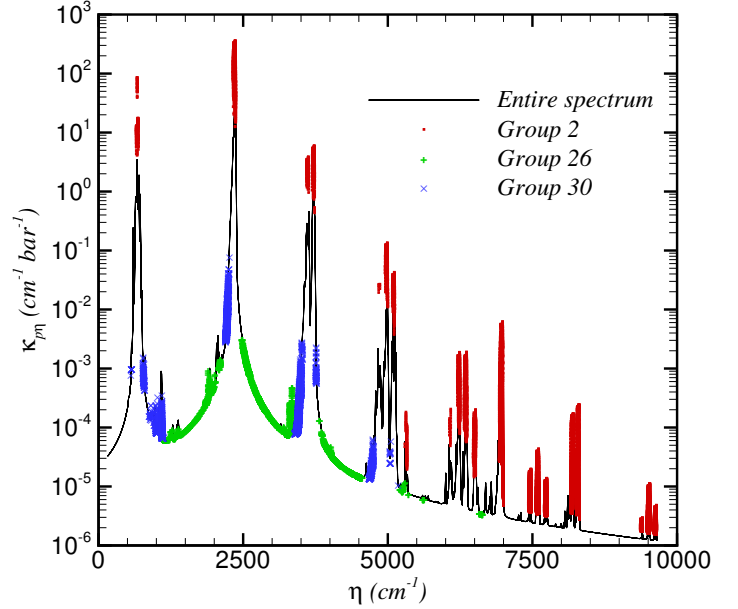


Figure 6. The absorption coefficient spectrum of CO₂ at 300 K and 1 bar, together with three typical spectral groups for CO₂.

minimizes

$$\sum_{j=1}^J \left[u(T_j, x_0; T_0, x_0; \eta_j) - u_m(T_j, x_0; T_0, x_0) \right]^2 = \min. \quad (18)$$

Figure 6 shows the absorption coefficient spectrum of CO₂ at 300 K and 1 bar, together with which spectral locations are sorted into three typical spectral groups for CO₂. The (red) square symbols are the absorption coefficients of Group 2, which is a group dominated by “cold” lines, usually making up the center of a band. Group 30 is shown as (blue) × symbols in Fig. 6, representing a group dominated by “hot” lines, generally located in the band wings. Finally, the (green) + symbols are the absorption coefficients of Group 26, which is dominated by “cold” lines at low temperatures, with “hot” lines waking up at an intermediate temperature, as shown in Fig. 5; such behavior is found in the low-absorption regions between bands. Note that, once determined, all spectral locations stay in their specific group, independent of the local state of the gas, ϕ . The same scheme for spectral grouping can be applied to other absorbing gases [16].

The full-spectrum k -distributions and their inverse $k_m(T_0, \phi, g_m)$ may now be calculated for each group and all states ϕ . Making the assumption of correlated absorption coefficients, these distributions may be compared with those

evaluated at the standard state ϕ_0 , leading to

$$u_{mg}(\phi, \phi_0, g_m) = \frac{k_m(T_0, \phi, g_m)}{k_m(T_0, \phi_0, g_m)}. \quad (19)$$

As an example, these scaling functions, for $\phi = (2000\text{K}, 1\text{bar}, 10\%)$ and $\phi_0 = (300\text{K}, 1\text{bar}, 10\%)$, are shown in Fig. 7 for all 32 spectral groups of CO₂. Note that, for each spectral group, the cumulative k -distribution ranges from a $g_{m,\min}$ to 1. A large range of $(1 - g_{m,\min})$ indicates that group m occupies a large part of the (Planck function weighted) spectrum. All ranges summed together must add to unity. Not surprisingly, the g -dependence of these scaling functions is weak: because of grouping criteria, the scaling function for each wavenumber comprising group m should have a scaling function closely following $u_m(\phi, \phi_0)$, i.e., should be independent of g_m . Therefore, at the 32-group level, we may assume the absorption coefficient not only to be correlated, equation (1), but scaled, obeying equation (2),

$$\kappa_\eta(\phi, \eta) = \kappa_\eta(\phi_0, \eta) u_m(\phi, \phi_0), \eta \in [\eta_m]. \quad (20)$$

This will allow the construction of a much more compact database with little additional loss of accuracy. The standard state for the database is taken as $\phi_0 = (T_0 = 1500\text{K}, p_0 =$

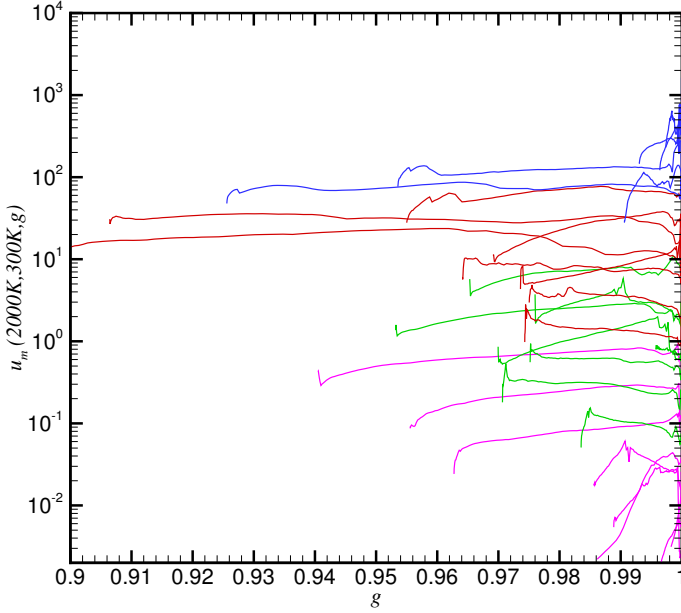


Figure 7. Variation of scaling function $u_m(2000\text{K}, 300\text{K}, g)$ with cumulative k -distribution g for CO_2 base groups.

1bar, $x_0 = 0.1$) simply for convenience, and should not be confused with the reference state (ϕ_{ref}) needed in equation (9) to recast the RTE as a function of cumulative k -distribution. Since the absorption coefficient is databased as scaled values at the 32-group level, the choice of reference state for 32GFSCK model is arbitrary. However, when groups are combined, the resulting absorption coefficient is no longer scaled, and an optimal choice for a reference state becomes important.

With 32 groups for CO_2 and the Planck function temperature ranging from 300K to 2500K (23 temperatures), 32×23 k -distributions, $k_m(T, \underline{\phi}_0, g_m)$ ($m = 1, \dots, 32$) have been evaluated and databased. The k -distributions at any nonstandard state $\underline{\phi}$ can then be calculated as

$$k_m(T, \underline{\phi}, g_m) = k_m(T, \underline{\phi}_0, g_m) u(\underline{\phi}, \underline{\phi}_0) \quad (21)$$

For most groups, the preassigned values for A_m, E_m and n_m are sufficient for use in equation (20); however, for a few groups the differences between u_{mg} [from equation (19)] and u_m [from equation (16)] were large enough to call for slight adjustments. This was done by first finding average scaling functions

$$\langle u_m \rangle(\underline{\phi}, \underline{\phi}_0) = \frac{\int_{g_{m,\min}}^1 u_{gm}(\underline{\phi}, \underline{\phi}_0, g_m) w(g_m) dg_m}{\int_{g_{m,\min}}^1 w(g_m) dg_m}, \quad (22)$$

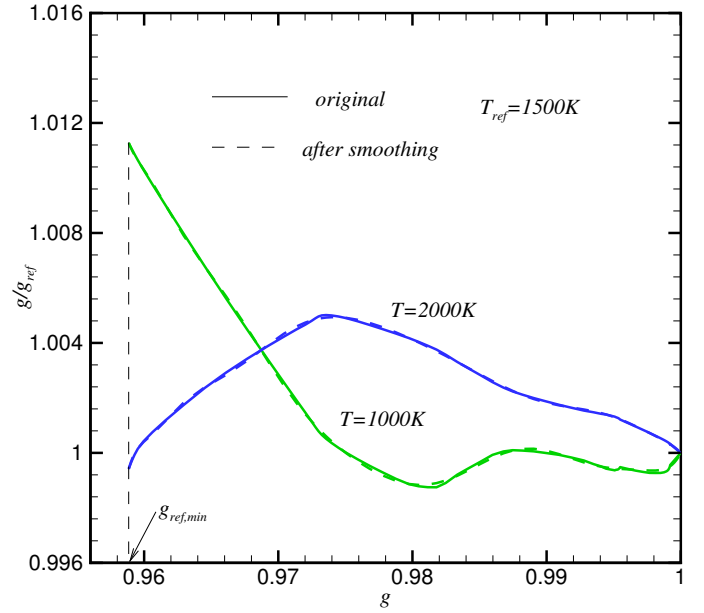


Figure 8. Original and smoothed cumulative k -distribution stretching factor g/g_{ref} .

where $w(g_m)$ is a weight function (set to unity in our calculations). This is followed by adjusting the values for A_m, E_m and n_m to minimize the function

$$\int_T \int_x (u_m - \langle u_m \rangle)^2 dx dT = \min. \quad (23)$$

Weight Function a

For each of the 32 spectral groups for CO_2 , the full-spectrum k -distributions can be calculated and databased. The required number of data points and, thus, the efficiency of the database is greatly affected by the smoothness of the weight function a defined in equation (11). This function is the ratio of two k -distributions, or, the ratio of the slopes of two cumulative k -distributions (evaluated at Planck function temperatures of T and T_{ref} , respectively). Therefore, the weight function is very sensitive to the structure of the k -distributions, (even though its behavior is much better than that of f itself [11]). Noisy weight functions will have detrimental effects on quadrature efficiency, in particular for groups with holes (ranges of absorption coefficient not present in the spectral group under consideration) in their k -distributions. Therefore, the k -distributions were smoothed, in order for them to produce smoothly varying weight functions a . This was achieved by first smoothing $g_m(T, \underline{\phi}_0, k)/g_{m,0}(T_0, \underline{\phi}_0, k)$, since a in equation (11) is evaluated as $dg_m/dg_{m,\text{ref}}$ (at identical values of k), where $\underline{\phi}_0 = (T_0 = 1500\text{K}, p_0 = 1\text{bar}, x_0 = 0.1)$ is the database standard state. Since the weight functions a are stretch-

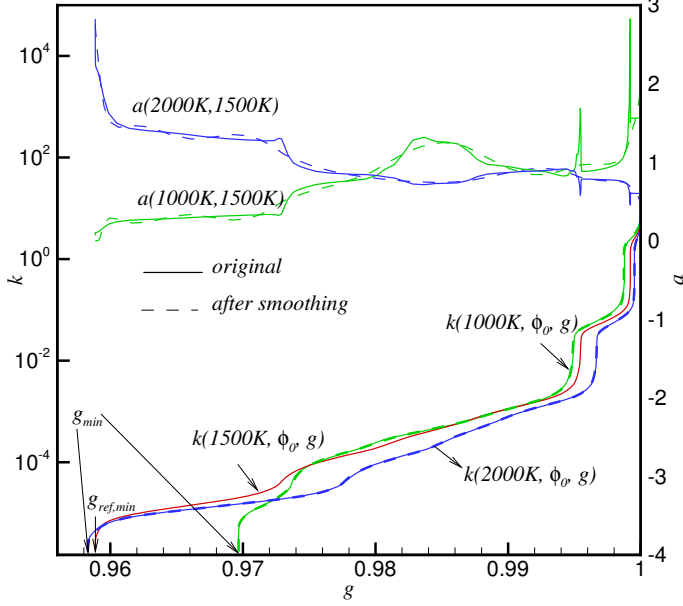


Figure 9. Original and smoothed weight functions a and cumulative k -distributions.

ing factors for the cumulative k -distribution at different Planck function temperatures, it is important to preserve the following integral during the smoothing process:

$$\int_{g_{m,0,\min}}^1 adg_{m,0} = \int \frac{dg_m}{dg_{m,0}} dg_{m,0} = \int_{g_{m,\min}}^1 dg_m = 1 - g_{m,\min} \quad (24)$$

Fig. 8 shows the original and smoothed $g_{14}(2000K, \underline{\phi}_0, k)/g_{14,0}(1500K, \underline{\phi}_0, k)$ and $g_{14}(1000K, \underline{\phi}_0, k)/g_{14,0}(1500K, \underline{\phi}_0, k)$ for Group 14 of CO_2 , whose unsmoothed a function is very noisy, especially near holes in the k -distribution. A smoothed k -distribution, for nonstandard conditions, can then be calculated from the standard k -distribution as

$$g_m^{(s)}(T, \underline{\phi}_0, k) = g_{m,0}(T_{\text{ref}}, \underline{\phi}_0, k) \left(\frac{g_m}{g_{m,0}} \right)^{(s)}, \quad (25)$$

where (s) stands for ‘‘smoothed values’’. Figure 9 shows the k -distributions at different Planck function temperature and the corresponding a function for Group 14 of CO_2 , with the absorption coefficient evaluated at $\underline{\phi}_0$. It can be seen that a very small change in the k -distribution function (nearly indiscernible) results in a much smoother a function.

Since different absorption coefficient regions may become important at different optical thicknesses, the database for the

32 groups of CO_2 was constructed with 100 k -boxes (values), allowing the user to choose proper quadrature points, depending on the problem at hand. With 32 groups, and 23 Planck function temperatures and 100 k -boxes (values) for each group, the size of the database is about 1 Megabyte.

Combination of Spectral Groups

For greater numerical efficiency (accompanied by a slight loss of accuracy), the spectral groups from the database can be combined to obtain coarser group models ($N = 1, 2, 4, \dots$). While the absorption coefficient can be assumed to be scaled at the the 32 group level, this is clearly not true after combining groups, unless a new scaling function is determined after each grouping, following the guidelines of Modest and Zhang [11]. However, if we simply assume that each group has a correlated absorption coefficient, then, since there is no overlap between different spectral groups, the k -distributions are additive, and one obtains

$$f_n(T_P, \underline{\phi}, k) = \sum_{m=m_{\min}(n)}^{m_{\max}(n)} f_m(T_P, \underline{\phi}, k), \quad (26)$$

where n is the new group resulting from combining a number of basic groups. Since each nonoverlapping group is populated only across $g_{\min} < g < 1$, the cumulative k -distribution for the combined group becomes

$$\begin{aligned} \int_k^\infty f_n(T_P, \underline{\phi}, k) dk &= \int_k^\infty \sum_m f_m(T_P, \underline{\phi}, k) dk \\ &= \sum_m \int_k^\infty f_m(T_P, \underline{\phi}, k) dk \end{aligned} \quad (27)$$

or

$$1 - g_n = \sum_m (1 - g_m) = N_n - \sum_m g_m, \quad N_n = m_{\max}(n) - m_{\min}(n) + 1 \quad (28)$$

i.e.,

$$g_n(T_P, \underline{\phi}, k) = \sum_m g_m(T_P, \underline{\phi}, k) - N + 1. \quad (29)$$

This relation may be inverted to give k_n as a function of the combined group’s cumulative k -distribution g ,

$$k_n(T_P, \underline{\phi}, g_n) = g_n^{-1}(T_P, \underline{\phi}, k_n). \quad (30)$$

This is demonstrated in Fig. 10, where Groups 3 and 4 were combined and the combined k -distribution essentially coincides with

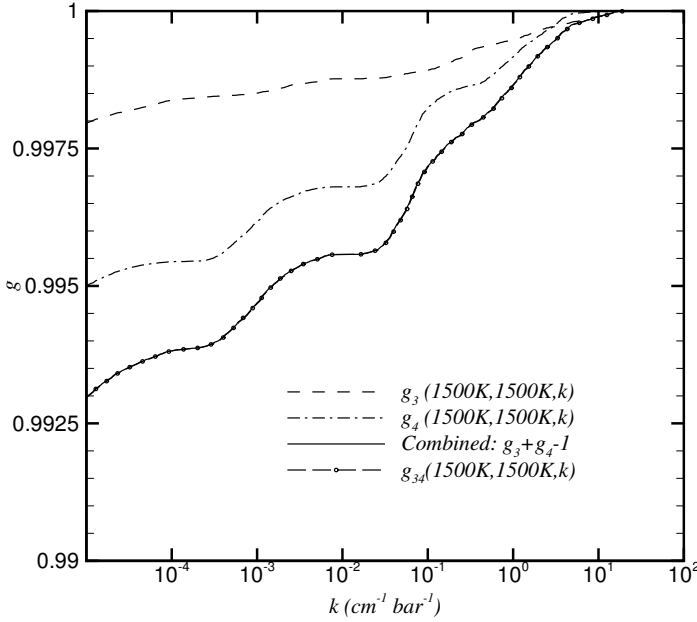


Figure 10. Combination of two spectral groups into one (CO₂ groups 3 and 4).

the k -distribution calculated directly from the HITEMP database [the only errors coming from the scaling in equation (21) and the smoothing of equation (25)].

Use of the Database

Solving a general radiation problem using N different spectral groups requires the solution of the RTE, equation (9), for each of the M spectral groups. This in turn, requires (i) definition of an optimal global reference state $\underline{\phi}_{\text{ref}}$, at which the absorption coefficient and its k -distribution are calculated “exactly”; (ii) precalculation of a set of k -distributions $k_m(T_{\text{ref}}, \phi, g_m)$ for each group, i.e., absorption coefficient evaluated at local state ϕ , Planck function at T_{ref} , and (iii) precalculation of a set of k -distributions $k_m(T, \underline{\phi}_{\text{ref}}, g_m)$ for each group, i.e., absorption coefficient evaluated at the reference state $\underline{\phi}_{\text{ref}}$, Planck function at local temperature T (for the evaluation of the weight function a). These distributions are extracted from the database as follows:

Step 1: A global reference state is chosen along the guidelines of Modest and Zhang [11], i.e., the Planck mean temperature as reference temperature and the volume-averaged mole fraction as reference mole fraction.

Step 2: Keeping in mind that the database uses a standard state of $\underline{\phi}_0 = (1500\text{K}, 1\text{bar}, 10\%)$, one finds for each of the 32 groups

$$k_m(T, \underline{\phi}, g) = k_m(T, \underline{\phi}_0, g) u_m(\underline{\phi}, \underline{\phi}_0). \quad (31)$$

At this point $k_m(T, \underline{\phi}, g)$ is available for all Planck function temperatures (including T_{ref}) and local states $\underline{\phi}$ (including $\underline{\phi}_{\text{ref}}$) in the form of 100 pairs of points $(k_{m,i}, g_{m,i})$.

Step 3: If groups are to be combined into an N -group model for greater numerical efficiency, this is now done through the use of equation (29). In the database, groups are numbered in such a way that groups with similar scaling function u_m are always next to each other, so adjacent groups should be combined. This results in 100 pairs of points $(k_{n,i}, g_{n,i})$ for the N combined groups.

Step 4: For all Planck function temperatures T , the weight functions $a_n(T, T_{\text{ref}}, g_n)$ are calculated from

$$a_{n,i} = \left. \frac{dg_n(T, \underline{\phi}_{\text{ref}})}{dg_n(T_{\text{ref}}, \underline{\phi}_{\text{ref}})} \right|_{k=k_{n,i}} \approx \frac{g_{n,i+1}(T, \underline{\phi}_{\text{ref}}) - g_{n,i-1}(T, \underline{\phi}_{\text{ref}})}{g_{n,i+1}(T_{\text{ref}}, \underline{\phi}_{\text{ref}}) - g_{n,i-1}(T_{\text{ref}}, \underline{\phi}_{\text{ref}})}. \quad (32)$$

Step 5: A set of J quadrature points, say $J = 10$, is chosen for the problem at hand to eventually carry out the integration in equation (14) as

$$I = \sum_n I_n = \sum_n \int_0^1 I_{g,n} dg_n \approx \sum_n \sum_{j=1}^J w_j I_{g,n}(g_{n,j}), \quad (33)$$

where the w_j and $g_{n,j}$ are quadrature weights and points, respectively. For this operation, the data sets for $k_n(T_{\text{ref}}, \phi, g_n)$ and $a_n(T, T_{\text{ref}}, g_n)$ are reduced to the corresponding J values each.

Step 6: Given the necessary set of k_n and a_n values, the RTEs for each of the n groups are solved and results collected according to equation (33).

SAMPLE CALCULATIONS

The Multi-Group approach and the 32-group database for CO₂ are tested in this section by considering several one-dimensional slabs of gas mixtures with varying temperatures and mole fractions. A uniform mixture of 10% CO₂–90% N₂ (by volume) at 1 bar, confined between two infinite parallel, cold and black plates, is considered first to test the validity of the model in situations of extreme temperature changes. An isothermal hot layer of 2000K with a fixed width of 50cm is adjacent to an isothermal cold layer at 300K of varying width. The radiative heat flux exiting the cold column is studied and is shown in Fig. 11, with LBL calculations serving as benchmark. For simplicity, a simple trapezoidal rule was used in the LBL calculations (with a resolution of 0.01cm⁻¹) and the accuracy of the LBL results should be expected to be within ≈1%. The Multi-Group FSCCK results calculated directly from the HITEMP database are shown by lines, while the symbols represent results using the 32-group database for CO₂, which assumes a scaled absorption coefficient at the 32 group level. The 32-group model, with its scaled absorption coefficient, is independent of

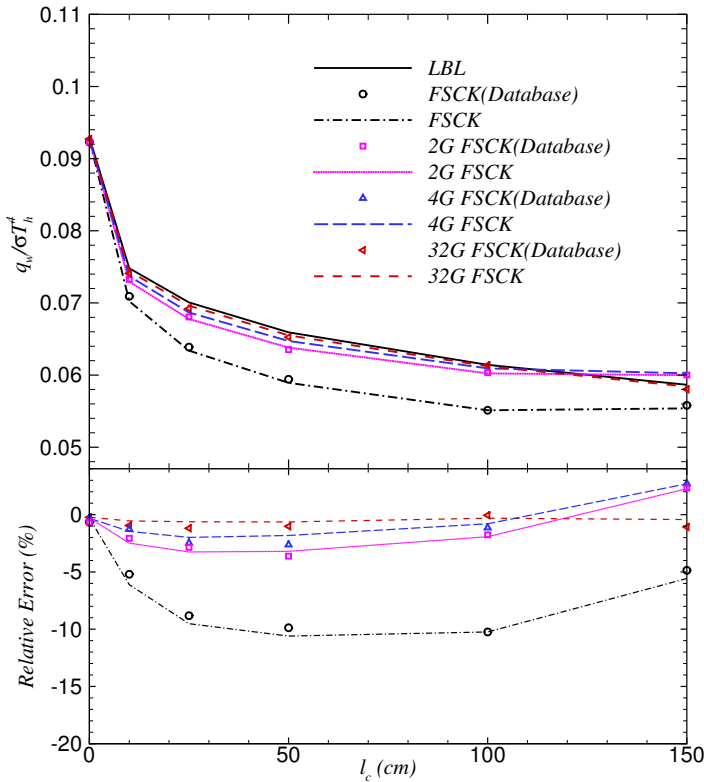


Figure 11. Radiative flux exiting from the cold column of a two-column CO₂-nitrogen mixture at different temperatures ($T_{\text{hot}} = 2000\text{K}$, $l_{\text{hot}} = 50\text{cm}$; $T_{\text{cold}} = 300\text{K}$, l_{cold} variable; uniform $p = 1\text{bar}$, $x_{\text{CO}_2} = 0.1$, cold and black walls on both sides) and their relative error compared with the LBL benchmark.

the choice of reference state, while for combined group, the reference state recommended by Modest and Zhang [11] was used. As can be seen from Fig. 11, the direct FSKC results and those from the database are in very good agreement. Note that there is a substantial improvement when going from a single group model (FSKC) to a 2GFSKC model, with the maximum error changing from 11% to less than 4%. The improvement from 2GFSKC to 4GFSKC is not as large and LBL accuracy can essentially be achieved with 8 or more groups (within the limits of quadrature error for both LBL and FSKC).

The next example considers a CO₂-N₂ gas mixture with both a step in temperature and a step in mixture ratio. The medium is again a one-dimensional slab with a hot layer (2000K, 20% CO₂, 50cm width) adjacent to a cold layer (300K, 50% CO₂, with varying cold layer l_c). The wall next to the hot layer is at 1000K and that next to the cold layer is at 0K, with both walls black. The radiative heat flux exiting the cold column of this mixture is shown in Fig. 12, leading to the same conclusions as the results of Fig. 11. A number of other cases were studied

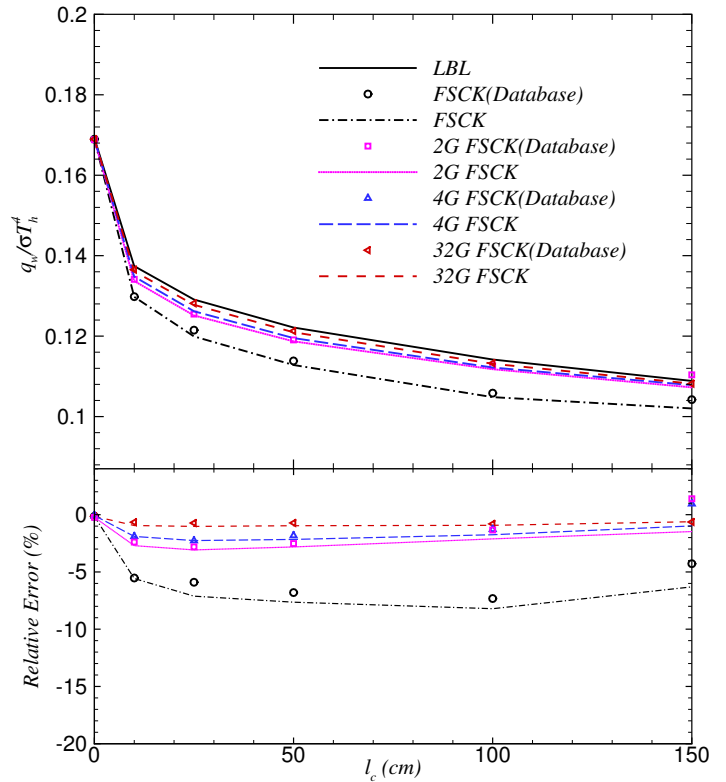


Figure 12. Same as Fig. 11, except that $x_{\text{hot}} = 0.2$, $x_{\text{cold}} = 0.5$ and the left wall is at 1000K.

and the same conclusions can be drawn: a substantial improvement occurs when going from a single group model to a 2GFSKC model; LBL accuracy can be approached with 8 or more groups.

SUMMARY AND CONCLUSIONS

A multi-Group Full-Spectrum Correlated k -distribution model (MGFSKC) has been developed, in which the spectral locations are broken up into M spectral groups, based on their absorption coefficient dependence on (partial) pressure and temperature. Like all k -distribution based methods, the MGFSKC model can be used with any desired RTE solution method. Like all global models, the MGFSKC method is limited to gray scattering and gray walls. A 32-group database based on HITEMP was built for CO₂ and tested for problems with large temperature gradients and sharp mole fraction changes. It was found that the MGFSKC model and the CO₂ database provides very accurate results for radiative heat transfer calculations and LBL accuracy can be approached at very affordable cost. While LBL calculations may need 1 million spectral calculations, the Multi-Group approach needs only 10-15 [spectral calculations] \times M [number of groups used]. The database for CO₂ has a size of 1 Megabyte

and is available upon request.

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