

Hybrid Full-Spectrum Correlated k -Distribution Method for Radiative Transfer in Nonhomogeneous Gas Mixtures

Gopalendu Pal
Michael F. Modest¹
Fellow ASME
e-mail: mfmolest@psu.edu

Liangyu Wang
Department of Mechanical and Nuclear
Engineering,
The Pennsylvania State University,
University Park, PA 16802

The full-spectrum k -distribution (FSK) approach is a promising model for radiative transfer calculations in participating media. FSK achieves line-by-line (LBL) accuracy for homogeneous media at a tiny fraction of LBL's high computational cost. However, inhomogeneities in gas temperature, total pressure, and component-gas mole fractions change the spectral distribution of the absorption coefficient and can cause inaccuracies in the FSK approach. In this paper, a new hybrid FSK method is proposed that combines the advantages of the multigroup FSK (MGFSK) method for temperature inhomogeneities in a single gas species and the multiscale FSK (MSFCK) method for concentration inhomogeneities in gas mixtures. In this new hybrid method, the absorption coefficients of each gas species in the mixture are divided into M spectral groups depending on their temperature dependence. Accurate MGFSK databases are constructed for combustion gases, such as CO_2 and H_2O . This paper includes a detailed mathematical development of the new method, method of database construction, and sample heat transfer calculations for 1D inhomogeneous gas mixtures with step changes in temperature and species mole fractions. Performance and accuracy are compared to LBL and plain FSK calculations. The new method achieves high accuracy in radiative heat transfer calculations in participating media containing extreme inhomogeneities in both temperature and mole fractions using as few as $M=2$ spectral groups for each gas species, accompanied by several orders of magnitude lower computational expense as compared to LBL solutions. [DOI: 10.1115/1.2909612]

Keywords: thermal radiation, k -distribution method, inhomogeneous gas mixture, multi-scale approach, global method

Introduction

Radiative transfer calculations in participating media can be most accurately evaluated by the line-by-line (LBL) approach, but, due to irregular gas phase absorption coefficients that rapidly vary across the spectrum, the radiative transfer equation (RTE) must be solved for up to 1×10^6 wavenumbers. Hence, the LBL approach is extremely time consuming and requires large computer resources. On the other hand, the absorption coefficient can be reordered into a monotonically increasing function, such that only a small number of quadrature point evaluations of the RTE is required [1,2], greatly reducing the computational cost. Several models have been proposed to apply the concept of reordering the absorption coefficient to the entire spectrum and these include the spectral-line-based weighted-sum-of-gray-gases (SLW) model [3,4], the absorption distribution function (ADF) method [5,6], and the recent full-spectrum k -distribution (FSK) method [7]. Whereas SLW and ADF methods are approximate schemes, in which the absorption coefficient is reduced to a few discrete values, the FSK method is an exact method for a correlated absorption coefficient using a continuous k -distribution over the entire spectrum. The FSK method achieves LBL accuracy for homogeneous media at a tiny fraction of LBL's computational cost. Since its introduction, the FSK method has undergone several major

developments [7–10] and has become one of the most popular spectral models for radiative transfer calculations.

Although the FSK scheme is an exact method for radiative calculations in homogeneous media, its application in strongly inhomogeneous emitting-absorbing media challenges its accuracy. Inhomogeneities in total pressure, temperature, and component mole fraction (partial pressure) alter the local spectral behavior of the absorption coefficient, which is critical in the FSK reordering process. The effect of strong variations in total pressure along with negligible variation in temperature produces only a small change in the k -distribution as evidenced in meteorological applications [1,11,12]. On the other hand, varying temperature and gas concentrations have substantial effects on the accuracy of k -distribution and FSK methods [7,11,13–15].

In order to address the inhomogeneity problem, several strategies with different levels of sophistication and accuracy have been proposed in the literature. All the commonly used strategies include either the assumption of a correlated absorption coefficient or the scaling assumption. Details of these two approaches can be obtained from Modest [8]. The application of both the correlated and scaled approaches to the FSK method leads to the full-spectrum correlated k -distribution (FSCK) and scaled k -distribution (FSSK) methods, respectively. To alleviate the inaccuracies in inhomogeneous media, two different approaches have been proposed, namely, the fictitious gas (FG) [6] or multiscale [9] approach and the multigroup (MG) approach [10,16]. The concept behind these two approaches is to break up the gas absorption coefficients into pieces that are as correlated or scaled as possible. In the FG approach, the individual spectral lines comprising the absorption coefficient are placed into separate scales based on

¹Corresponding author.

Contributed by the Heat Transfer Division of ASME for publication in the JOURNAL OF HEAT TRANSFER. Manuscript received May 29, 2007; final manuscript received October 16, 2007; published online June 3, 2008. Review conducted by Walter W. Yuen.

their temperature dependence. In the MG approach, spectral positions, i.e., wavenumbers, are placed into several groups according to their dependence on temperature and partial pressure. Both approaches achieve increased correlation in the absorption coefficient within each FG or spectral groups and improve the accuracy of radiative calculations in inhomogeneous media. The multigroup FSK (MGFSK) method has been shown to achieve great accuracy for a single gas species with inhomogeneity in temperature [9,10,16], whereas the multiscale FSK (MSFSK) method can efficiently treat mixtures of absorbing gases with severe species inhomogeneity [17]. However, challenges still remain for radiative calculations in a gas mixture containing both temperature and species concentration inhomogeneities.

FSK calculations are very accurate and time efficient provided the required FSKs are known, which are tedious to compile from spectroscopic databases, such as HITRAN [18], HITEMP [19], and CDSD-1000 [20]. Several very approximate correlations have been generated by Denison and Webb [3,4] and Modest et al. [7,9,10,16]. However, to make accurate FSK calculations feasible for general engineering purposes, preassembled FSK must be available in the form of accurate and compact databases. Full-spectrum MG databases have been constructed by Zhang and Modest for carbon dioxide and water vapor from the HITEMP spectroscopic database [10,16]. The spectral positions of each gas were placed into 32 exclusive spectral groups depending on their temperature and partial pressure dependence. The absorption coefficients at the 32 group level satisfy the scaling approximation. The spectral groups from the databases are scalable, i.e., for better numerical efficiency, the spectral groups can be combined to obtain coarser numbers of groups. It has been reported that close-to-LBL accuracy can be achieved by considering only four such groups, within which the assumption of a correlated absorption coefficient holds.

In the current paper, a new hybrid multiscale multigroup FSK (MSMGFSK) method is proposed, which is capable of accurately handling radiative transfer in a gas mixture containing both temperature and partial pressure inhomogeneities with/without gray wall emission. The medium may also contain gray particles. However, mixtures containing nongray particles are beyond the scope of the present paper, because mixing of species for such case cannot be accurately performed at the full-spectrum level. This requires a narrow-band database and will be addressed in a follow up paper. The present MSMGFSK method resolves the absorption coefficient of an individual species in a mixture as one of its scales. Within each scale, the wavenumbers are placed into exclusive spectral groups according to their temperature dependence. Mixing of species is addressed by introducing an overlap parameter to approximate the effect of overlap among scales. In the MG databases created by Zhang and Modest [10,16], the absorption coefficients were obtained from the HITEMP spectroscopic database. Unfortunately, it has been observed that the HITEMP database is not accurate for CO₂ at temperatures higher than 1000 K [20,21]. Thus, also a new and better correlated database is constructed with spectral absorption coefficients for water vapor calculated from HITEMP 2000 and for carbon dioxide from CDSD-1000, which is considered more reliable. Since it had been found that radiative calculations using four groups can achieve close-to-LBL accuracy with faster computational times [10,22], MG databases are constructed with only four such groups. Sample calculations are performed for gas mixtures with temperature and partial pressure inhomogeneities. For all cases, results are compared to FSK and LBL calculations.

Hybrid MSMGFSK Approach

Although the multiscale multigroup full-spectrum correlated k -distribution (MSMGFSK) method can be easily extended to include gray absorbing and scattering particles, for brevity, a medium consisting of a mixture of molecular gases is considered and the RTE for this medium can be written as [23]

$$\frac{dI_\eta}{ds} = \kappa_\eta(\underline{\phi})(I_{b\eta} - I_\eta) \quad (1)$$

subject to the boundary condition

$$\text{at } s = 0: \quad I_\eta = I_{w\eta} \quad (2)$$

Here, I_η is the spectral radiative intensity, κ_η is the absorption coefficient, $I_{b\eta}$ is the spectral blackbody intensity (or Planck function), and wavenumber η is the spectral variable. The term $\underline{\phi}$ is a vector of state variables that affect κ_η , which include temperature T , total pressure P , and gas mole fractions \underline{x} : $\underline{\phi} = (T, P, \underline{x})$. The boundary intensity $I_{w\eta}$ may be due to emission and/or reflection from the enclosure wall [24].

The total absorption coefficient κ_η is first separated into contributions from N component gases, e.g., CO₂ and H₂O, and then the spectral locations of the n th gas absorption coefficient are sorted into M exclusive spectral groups, i.e.,

$$\kappa_\eta = \sum_{n=1}^N \sum_{m=1}^{M_n} \kappa_{nm\eta} \quad I_\eta = \sum_{n=1}^N \sum_{m=1}^{M_n} I_{nm\eta} \quad (3)$$

and the radiative intensity I_η is accordingly broken up. Note that the spectral locations constituting the m th group may not be consecutive. The RTE is then transformed into $\sum_{n=1}^N M_n$ component RTEs, one for each group of each gas or scale:

$$\frac{dI_{nm\eta}}{ds} = \kappa_{nm\eta}(\underline{\phi})I_{b\eta} - \kappa_\eta(\underline{\phi})I_{nm\eta} \quad \text{for } n = 1, \dots, N, \quad m = 1, \dots, M_n \quad (4)$$

It is observed, physically, that the intensity $I_{nm\eta}$ is due to emission from the m th group of the n th gas specie (the nm th group) but subject to absorption by all groups of other gases plus its own group. There is no overlap among groups of a single species and, therefore, there is no emission over wavenumbers where $\kappa_{nq\eta}$ ($q \neq m$) absorbs. Thus, in Eq. (4),

$$\kappa_\eta = \kappa_{nm\eta} + \sum_{l \neq n}^N \sum_{q=1}^{M_l} \kappa_{lq\eta} \quad (5)$$

We now apply the FSK scheme [23] to the RTE of each group: First, Eq. (4) is multiplied by Dirac's delta function $\delta(k_{nm} - \kappa_{nm\eta}(\underline{\phi}_0))$, followed by division with

$$f_{nm}(T_0, \underline{\phi}_0, k_{nm}) = \frac{1}{I_{b\eta}(T_0)} \int_0^\infty I_{b\eta}(T_0) \delta(k_{nm} - \kappa_{nm\eta}(\underline{\phi}_0)) d\eta \quad (6)$$

where $\underline{\phi}_0$ and T_0 refer to a reference state. The resulting equation is then integrated over the entire spectrum, leading to

$$\frac{dI_{nm\eta}}{ds} = k_{nm} a_{nm} I_b - \lambda_{nm} I_{nm\eta} \quad \text{for } n = 1, \dots, N, \quad m = 1, \dots, M_n \quad (7)$$

where

$$I_{nm\eta} = \frac{\int_0^\infty I_{nm\eta} \delta(k_{nm} - \kappa_{nm\eta}(\underline{\phi}_0)) d\eta}{f_{nm}(T_0, \underline{\phi}_0, k_{nm})} \quad (8)$$

$$g_{nm} = \int_0^{k_{nm}} f_{nm}(T_0, \underline{\phi}_0, k) dk \quad (9)$$

$$a_{nm} = \frac{f_{nm}(T, \underline{\phi}_0, k_{nm})}{f_{nm}(T_0, \underline{\phi}_0, k_{nm})} \quad (10)$$

$$\lambda_{nm} I_{nm} = k_{nm} I_{nm} + \frac{\int_0^\infty (\sum_{l \neq n} \sum_{q=1}^{M_l} \kappa_{lq}(\phi)) I_{nm} \delta(k_{nm} - \kappa_{nm}(\phi_0)) d\eta}{f_{nm}(T_0, \phi_0, k_{nm})} \quad (11)$$

Here, the absorption coefficient within each group has been assumed to be correlated. This implies that $k_{nm} = k_{nm}(T_0, \phi, g_{nm})$ is evaluated from the k -distribution of the local absorption coefficient of the nm th group weighted by the Planck function at the reference temperature [23]. The second term in Eq. (7) is due to the overlap of the absorption coefficient of the nm th group, $\kappa_{nm\eta}$ with groups of all other gases, and this overlap only occurs over part of the spectrum. Physically, the overlap coefficient λ_{nm} is a reordered absorption coefficient of the nm th group taking into account the overlap with groups of all other gases. Based on the MSFSK approach, the λ_{nm} can be approximately determined since the overlap effects between groups are relatively small. There are many ways of approximating λ_{nm} . Here, the approach used in the original MSFSK development is followed, that is, the overlap coefficient λ_{nm} is determined in such a way that the emitted intensity emanating from a homogeneous layer bounded by cold black walls is predicted exactly [9].

In Eq. (7), the reordering is performed in terms of $\kappa_{nm\eta}$ and the overlap coefficient between $\kappa_{nm\eta}$ and κ_η during the reordering process is lumped into λ_{nm} . In order to determine λ_{nm} , the reordering can also be performed in terms of κ_η which, for a homogeneous layer at temperature T , leads to

$$\frac{dI_{nm}^*}{ds} = \frac{k_{nm}^* I_b}{f(T, \phi, k)} - k I_{nm}^* \quad \text{for } n = 1, \dots, N, \quad m = 1, \dots, M_n \quad (12)$$

where

$$f(T, \phi, k) = \frac{1}{I_b(T)} \int_0^\infty I_{b\eta}(T) \delta(k - \kappa_\eta(\phi)) d\eta \quad (13)$$

$$I_{nm}^* = \frac{\int_0^\infty I_{nm\eta} \delta(k - \kappa_\eta(\phi)) d\eta}{f(T, \phi, k)} \quad (14)$$

$$k_{nm}^* = \frac{1}{I_b(T)} \int_0^\infty I_{b\eta}(T) \kappa_{nm\eta} \delta(k - \kappa_\eta(\phi)) d\eta \quad (15)$$

In Eq. (12), the interaction between $\kappa_{nm\eta}$ and κ_η is lumped into k_{nm}^* . The solutions to Eqs. (7) and (12) for a homogeneous layer at temperature T bounded by cold black walls can be analytically obtained, and the total exiting intensities at $s=L$, obtained from Eqs. (7) and (12), respectively, are

$$I_{nm} = \int_0^1 I_{nm} dg = \int_0^\infty \frac{k_{nm}}{\lambda_{nm}} I_b [1 - \exp(-\lambda_{nm} L)] f_{nm}(T, \phi, k_{nm}) dk_{nm} \quad (16)$$

and

$$I_{nm}^* = \int_0^1 I_{nm}^* dg = \int_0^\infty \frac{k_{nm}^*}{k} I_b [1 - \exp(-kL)] dk \quad (17)$$

The spectrally integrated intensity, I_{nm} , must be equal to I_{nm}^* , and this requirement leads to

$$\lambda_{nm} = k \quad \text{and} \quad k_{nm} f_{nm}(T, \phi, k_{nm}) dk_{nm} = k_{nm}^*(k) dk \quad (18)$$

or

$$k_{nm}^*(\lambda_{nm}) d\lambda_{nm} = k_{nm} f_{nm}(T, \phi, k_{nm}) dk_{nm} \quad (19)$$

Equation (19) provides the relationship between λ_{nm} and k_{nm} that is required to solve Eq. (7). One convenient way of determining λ_{nm} is by using the relationship [9]

$$\int_0^{k_{nm}} k'_{nm} f_{nm}(T, \phi, k'_{nm}) dk'_{nm} = \int_0^{k'=\lambda_{nm}} k_{nm}^*(k') dk' \quad (20)$$

In wavenumber space, this can also be expressed as

$$\int_{\eta | \kappa_{nm\eta} \leq k_{nm}} \kappa_{nm\eta} I_{b\eta}(T) d\eta = \int_{\eta | \kappa_\eta \leq \lambda_{nm}} \kappa_{nm\eta} I_{b\eta}(T) d\eta \quad (21)$$

Equation (20) is an implicit relation for the $\lambda_{nm} - k_{nm}$ relationship. In practice, the left- and right-hand sides of Eq. (20) are evaluated for a set of predetermined k_{nm} and λ_{nm} values and the results are stored in two arrays. The corresponding λ_{nm} values for the k_{nm} values used in the RTE evaluations are determined by interpolation from the two arrays. The so-determined λ_{nm} will be a function of the state variables (i.e., temperature and gas species concentration) as well as k_{nm} (or g_{nm}).

Evaluation of Overlap Coefficient λ_{nm}

The left-hand side (LHS) of Eq. (20) can be readily evaluated since

$$\text{LHS} = \int_0^{g_{nm}(k_{nm})} k'_{nm} dg'_{nm} \quad (22)$$

and the $k_{nm} - g_{nm}$ distribution of the nm th group can be obtained from the MG databases. The right-hand side (RHS) of Eq. (20) contains the k_{nm}^* term, which may be directly calculated from Eq. (15) using high resolution spectroscopic databases, if the spectral locations of each spectral group are known. This direct calculation, however, is extremely tedious and impractical for the solution of general problems. It is desirable to evaluate the RHS of Eq. (15) using databased MG $k-g$ -distributions for faster and efficient computation. The MG database construction for combustion gases CO₂ and H₂O is discussed in detail in the following section.

In order to do so, the quantity Q_{nm} is considered for the nm th group:

$$Q_{nm} = \frac{1}{I_b} \int_0^\infty I_{b\eta} \kappa_{nm\eta} \exp(-\kappa_\eta L) d\eta \quad (23)$$

Physically, Q_{nm} is related to the emission from the nm th group, attenuated over path L by the groups of all other gases and itself. Q_{nm} can be rewritten as

$$Q_{nm} = \frac{1}{I_b} \int_0^\infty I_{b\eta} \kappa_{nm\eta} \int_0^\infty \exp(-kL) \delta(k - \kappa_\eta) dk d\eta = \int_0^\infty k_{nm}^* \exp(-kL) dk = \mathcal{L}(k_{nm}^*) \quad (24)$$

i.e., Q_{nm} is the Laplace transform of k_{nm}^* . Q_{nm} can also be written as

$$Q_{nm} = \frac{1}{I_b} \int_0^\infty I_{b\eta} \kappa_{nm\eta} \exp(-\kappa_{nm\eta} L) \prod_{l \neq n} \exp(-\kappa_{l\eta} L) d\eta \approx \frac{1}{I_b} \int_0^\infty I_{b\eta} \kappa_{nm\eta} \exp(-\kappa_{nm\eta} L) d\eta \times \prod_{l \neq n} \left(\frac{1}{I_b} \int_0^\infty I_{b\eta} \exp(-\kappa_{l\eta} L) d\eta \right) \quad (25)$$

where $\kappa_{l\eta}$ is the total (all groups) absorption coefficient of the l th gas species. The second step follows by recognizing that the integrator in the first step is a Planck function weighted averaging operator, together with the assumption that the absorption coefficients of the nm th group and all the other gases are statistically uncorrelated with each other. Since the mixing in Eq. (25) is at the full-spectrum level, it is expected to be somewhat less accurate than on a narrow-band level [25]. However, the uncorrelated assumption should be reasonable here since the nm th group not only comes from a different gas but also from scattered parts of the spectrum.

The k -distribution method can then be applied to Eq. (25), which is written as

$$\begin{aligned} Q_{nm} &\approx \int_0^1 k_{nm} \exp(-k_{nm}L) dg_{nm} \prod_{l \neq n} \left(\int_0^1 \exp(-k_l L) dg_l \right) \\ &= \int_{g_{nm}=0}^1 \left(\int_{\substack{g_l=0 \\ l \neq n}}^1 \cdots \int k_{nm}(g_{nm}) \right. \\ &\quad \left. \times \exp\left(-\sum_{l \neq n} k_l L - k_{nm}L\right) \prod_{l \neq n} dg_l \right) dg_{nm} \end{aligned} \quad (26)$$

Here, $k_l(g_l)$ is the k - g -distribution of the entire l th gas, obtained by combining all groups into one [10],

$$g_l(T, \phi, k) = \sum_{q=1}^M g_{lq}(T, \phi, k) - M + 1 \quad (27)$$

evaluated at any given k (same for all groups).

Equating Eqs. (26) and (24) leads to

$$\begin{aligned} \mathcal{L}(k_{nm}^*) &= \int_{g_{nm}=0}^1 \left(\int_{\substack{g_l=0 \\ l \neq n}}^1 \cdots \int k_{nm} \right. \\ &\quad \left. \times \exp\left(-\sum_{l \neq n} k_l L - k_{nm}L\right) \prod_{l \neq n} dg_l \right) dg_{nm} \end{aligned} \quad (28)$$

and the integral property of the Laplace transform gives

$$\begin{aligned} \mathcal{L}\left(\int_0^{k=\lambda_{nm}} k_{nm}^*(k) dk\right) \\ = \int_{g_{nm}=0}^1 \left(\int_{\substack{g_l=0 \\ l \neq n}}^1 \cdots \int k_{nm} \times \frac{\exp(-\sum_{l \neq n} k_l L - k_{nm}L)}{L} \prod_{l \neq n} dg_l \right) dg_{nm} \end{aligned} \quad (29)$$

Finally, taking the inverse of the Laplace transformation results in

Table 1 Precalculated gas states and reference temperatures

Parameter	Sampling	Number of samples
Species	CO ₂ and H ₂ O	2
Total pressure	0.1–0.5 bar every 0.1 bar; 0.7 bar; 1.0–14.0 bar every 1.0 bar; 15.0–30.0 bar every 5.0 bar	24
Local gas temperature	300–2500 K every 100 K	23
Mole fraction	0.0–1.0 every 0.25	5
Planck function temperature	300–2500 K every 100 K	23

$$\begin{aligned} \text{RHS} &= \int_0^{k=\lambda_{nm}} k_{nm}^*(k) dk \\ &\approx \int_{g_{nm}=0}^1 \left(\int_{\substack{g_l=0 \\ l \neq n}}^1 \cdots \int k_{nm} H\left(k - \sum_{l \neq n} k_l - k_{nm}\right) \prod_{l \neq n} dg_l \right) dg_{nm} \end{aligned} \quad (30)$$

where H is the Heaviside step function.

By equating the LHS and RHS, a generic expression is obtained for the determination of the overlap coefficient λ_{nm} based on group k -distributions constructed from the MG databases, i.e.,

$$\begin{aligned} \int_0^{g_{nm}(k_{nm})} k_{nm}' dg_{nm}' \\ = \int_{g_{nm}=0}^1 \left(\int_{\substack{g_l=0 \\ l \neq n}}^1 \cdots \int k_{nm} H\left(\lambda_{nm} - \sum_{l \neq n} k_l - k_{nm}\right) \prod_{l \neq n} dg_l \right) dg_{nm} \end{aligned} \quad (31)$$

The number of multiple integrals on the RHS of Eq. (31) is N , the number of component gases in the mixture.

Multigroup Database Construction

As stated earlier, accurate and compact databases of MGFSKs are constructed as a part of this work. The spectral absorption coefficients for water vapor are calculated from HITEMP 2000 and for carbon dioxide CDS-1000 is used, which is considered more reliable than HITEMP for temperatures higher than 1000 K [20,21], as assembled by Wang and Modest [26]. The resulting MG k - g -distributions of the combustion gases are stored for various values of total pressure, local gas temperature, species mole fraction, and Planck function temperature and are summarized in Table 1.

Grouping of Wavenumbers. The wavenumbers of each gas species in 0.01 cm⁻¹ intervals are grouped according to the temperature dependence of their absorption coefficients. Some typical results are shown in Figs. 1 and 2. Figure 1 corresponds to a few chosen spectral locations across the 4.3 μ m band of CO₂ in a mixture with 10% CO₂ and 90% N₂, while Fig. 2 corresponds to a few chosen spectral locations across the 2.7 μ m band of H₂O in a H₂O–N₂ mixture with 10% H₂O. It is observed that there are distinct behaviors of absorption coefficients with temperature, which are consistent for all spectral locations and gas species. This temperature dependence is classified into four categories and

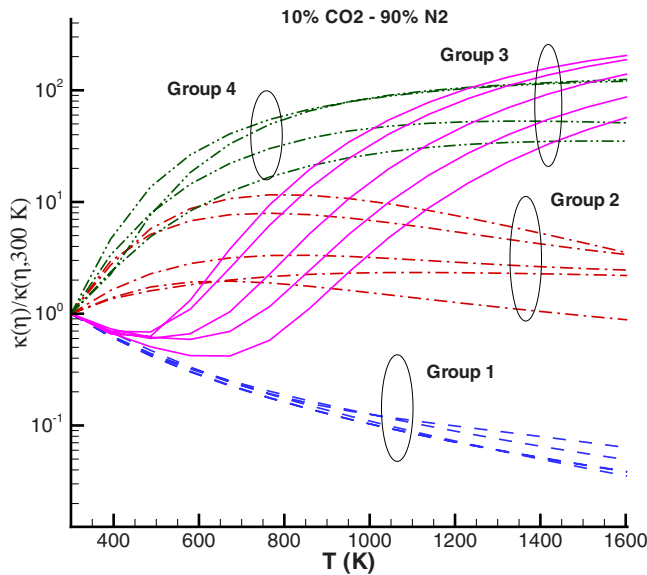


Fig. 1 Grouping of several spectral locations across 4.3 μm band of CO_2 in a CO_2 -air mixture containing 10% CO_2

used for initial grouping of the spectral locations.

Step 1. As seen from Figs. 1 and 2, lines with decreasing κ_η with temperature at all temperatures are collected into Group 1, those which have increasing κ_η at low temperature but then decrease later on are placed into Group 2, lines that first decrease but later on wake up are placed into Group 3, and finally the lines that wake up at low temperature and continue to rise are collected into Group 4.

Step 2. After this initial grouping, each group is assigned an average k -profile, which is expressed as

$$k_{ij} = \frac{\sum_\eta [\kappa_\eta(T)/\kappa_\eta(T_{\text{ref}})] \kappa_\eta(T_{\text{ref}}) I_{b\eta}(T_{\text{ref}})}{\sum_\eta \kappa_\eta(T_{\text{ref}}) I_{b\eta}(T_{\text{ref}})} = \frac{\sum_\eta \kappa_\eta(T) I_{b\eta}(T_{\text{ref}})}{\sum_\eta \kappa_\eta(T_{\text{ref}}) I_{b\eta}(T_{\text{ref}})} \quad (32)$$

where i is the counter-indicating group and j is the temperature. Unlike the database constructed by Zhang and Modest [10,16], a

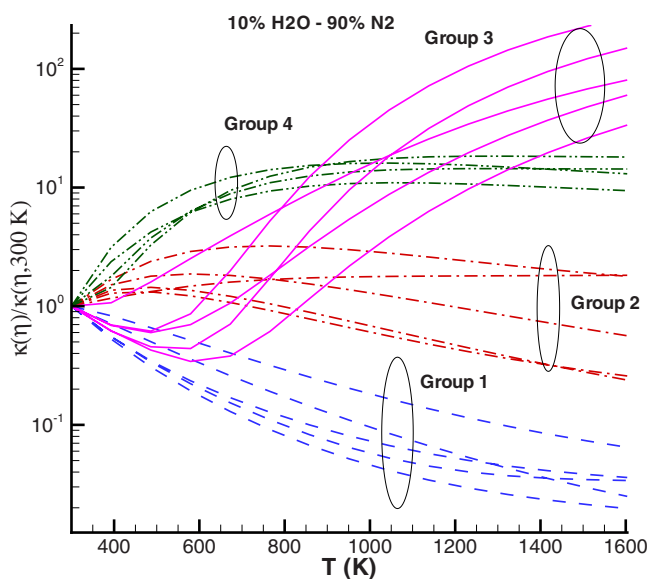


Fig. 2 Grouping of several spectral locations across 2.7 μm band of H_2O in a H_2O -air mixture containing 10% H_2O

weighted average of $\kappa_\eta(T)/\kappa_\eta(T_{\text{ref}})$ is employed, using spectral emission $\kappa_\eta(T_{\text{ref}}) I_{b\eta}(T_{\text{ref}})$ as the weight factor. In typical combustion applications, the maximum temperature is expected to vary between 500 K and approximately 1600 K, and for such temperature range, a value of $T_{\text{ref}}=850$ K was found to give the best grouping results.

The following are the steps used to optimize the grouping of wavenumbers:

Step 3. The group tag for each wavenumber is determined by minimizing the normalized departure of its relative temperature dependence from the average k -profile of the groups:

$$\sum_j \frac{(k_{ij} - C_{\eta i} \kappa_{\eta i})^2}{[\max(0.1 \kappa_{\eta, \text{max}}, k_{ij})]^2} = \varepsilon_{\eta i} \quad (33)$$

where

$$C_{\eta i} = \frac{\sum_j k_{ij} \kappa_{\eta i}}{\sum_j \kappa_{\eta i}^2} \quad (34)$$

In Eq. (33), the departure of the absorption coefficients from the average k -shape of the group is normalized in such a way that very low values of the absorption coefficient are given less importance. The numerator of Eq. (33) is the absolute departure of the absorption coefficient from the average k -shape, whereas the denominator normalizes that departure with respect to the average k -shape of the group. $C_{\eta i}$ is a constant optimized for each wavenumber, since the departure from the average k -shape is to be minimized, not departure from k itself. After calculating the total departure ($\varepsilon_{\eta i}$) from the average k -shape, the spectral locations are assigned to that group for which the value of $\varepsilon_{\eta i}$ is minimum.

Step 4. After regrouping, the average k -profile of each group is updated based on Planck function weighted absorption coefficients:

$$k_{ij} = \frac{\sum_\eta w_{\eta i} \kappa_{\eta i} C_{\eta i}}{\sum_\eta w_{\eta i}} \quad \text{where } w_{\eta i} = \kappa_\eta(T_{\text{ref}}) I_{b\eta}(T_{\text{ref}}) \quad (35)$$

and the process is repeated until less than 1% of the total number of wavenumbers change groups.

Once all spectral locations are grouped, the full-spectrum k - g distributions are calculated for each group and each gas species for the parameters presented in Table 1. When calculating FSKs for each group of a gas species, a set of nominal k -values between the group maximum and minimum k -values must be chosen at the local gas state. Here, a power law distribution of k -values is considered [26] and a total number of k -bins of $N_k=2000$. Details on the calculations of (MG) FSKs, and the weight function a from the absorption coefficients can be obtained from Zhang and Modest [7,10]. After calculating the initial k -distributions with 2000 k -bins, data compaction is performed using Gaussian quadrature schemes with a fixed- g concept as outlined by Wang and Modest [26]. The final database contains 128 k -distribution data points for each group. To eliminate the detrimental effect of noise in the stretch function a on quadrature efficiency, natural B -splines are used to smoothen the k - g -distributions by a small amount, resulting in better-behaved a -functions. Figure 3 shows the original and smoothened k - g -distributions and stretching functions a for Group 2 of a H_2O - N_2 mixture with 10% H_2O at 1500 K local gas temperature and 1000 K as the reference temperature. It is observed that a very small change (nearly indiscernible smoothening) in the k -distributions can result in a much smoother a -function.

The MG full-spectrum database is used to obtain the k - g -distributions for each group of each gas species. To obtain the k -distribution for an arbitrary state, interpolation is needed between precalculated states stored in the database. For a single gas species, the k -distribution is specified by total pressure (P), local gas temperature (T), mole fraction (x), and a Planck function temperature (T_0). Hence, for full-spectrum cases, four-dimensional

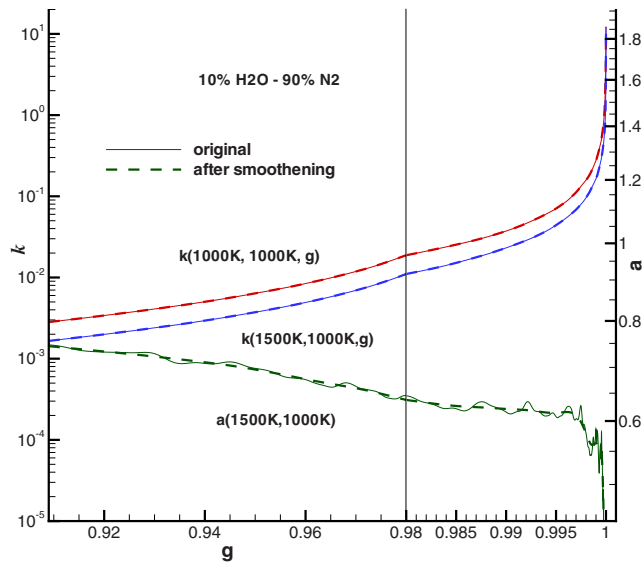


Fig. 3 Original and smoothed weight function a and cumulative k -distributions of Group 2 for 10% H_2O in H_2O -air mixture

interpolations in (P, T, T_0, x) are required. In order to achieve acceptable accuracy with small computational cost, a hybrid scheme is employed for database interpolation: 1D spline interpolation is used for P and trilinear interpolation for $T-T_0-x$ as proposed by Wang and Modest [26]. The MG database containing four groups for each gas species has a total size of 500 Mbytes. For a given state, MG $k-g$ -distributions can be obtained from the database in 20 ms on a Pentium Zeon 2.4 GHz computer.

The newly constructed MG database is scalable, i.e., for faster computation, the groups can be combined to obtain coarser groups. The $k-g$ -distributions of the combined group can be calculated [10] from Eq. (27) as

$$1 - g_n(k) = \sum_m (1 - g_m(k)) \quad (36)$$

where g_n and g_m are the cumulative k -distributions for the same k -values of the combined groups and original groups, respectively. Details of group combination can also be obtained from Zhang and Modest [10]. When groups are combined to obtain a two-group $k-g$ -distribution from four groups, the first two groups are combined into one group and the last two into second group, since the average characteristics of Groups 1 and 2 are similar (both of them contain lines with decreasing κ_η with increase in temperature at higher temperature). Groups 3 and 4 also have similarity in the sense that they contain lines with increasing κ_η at higher temperature.

Sample Calculations

To illustrate the performance of the newly created MG database in conjunction with the new hybrid MSMGFSCCK method in handling inhomogeneous gas mixtures, a few sample calculations with extreme temperature and mole-fraction (partial pressure) inhomogeneities are performed. In all cases, a one-dimensional medium containing CO_2 - H_2O - N_2 gas mixtures confined between cold black walls is considered. The mixture consists of two different homogeneous layers (denoted as left and right layers/columns) adjacent to each other. Two cases of total pressure, i.e., 1 bar and 10 bar, are considered. The left layer is at 1500 K and has a fixed width of 50 cm. The right layer is cold and at 300 K. The width of the cold layer is varied in the calculations. The radiative heat transfer leaving from the right layer is calculated using the LBL method, the single-scale FSCCK method, and the hybrid MSMGFSCCK method. For consistency, all three methods

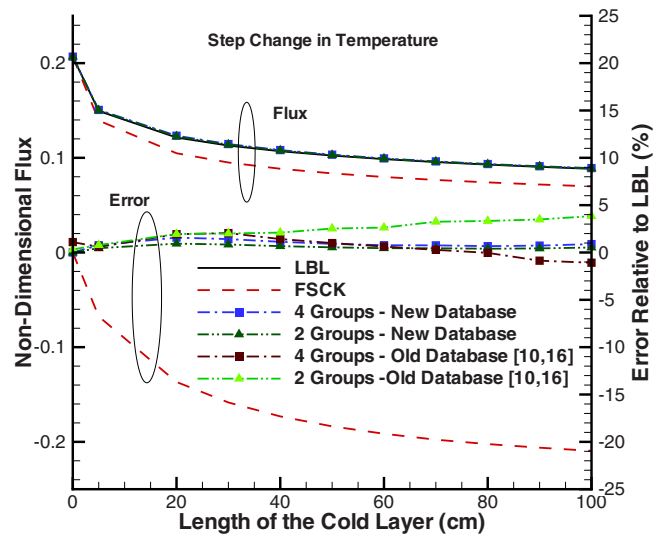


Fig. 4 Nondimensional heat flux leaving an inhomogeneous slab of 10% CO_2 and 20% H_2O at a total pressure of 1 bar with a step change in temperature: The hot left layer is at 1500 K and the cold right layer is at 300 K

employ absorption coefficients obtained from CSDS-1000 and HITEMP for CO_2 and H_2O , respectively. In the MSMGFSCCK calculations, the required $k-g$ -distributions are obtained by interpolating the database, while in the single-scale FSCCK calculations, the required $k-g$ -distributions are directly calculated from the absorption coefficients without mixing k -distribution of species, i.e., the absorption coefficients are calculated for the mixture before the k -distributions are formed. For all k -distribution calculations, ten quadrature points (g -values) were employed. It was found that using more than ten quadrature points resulted in negligible improvement. Therefore, a total number of 10 (g -values) \times 2 (species) \times 2 or 4 (groups) = 40 or 80 RTE evaluations was required for each case.

The LBL calculations serve as benchmark and the FSCCK calculations serve to demonstrate the improvement made by the hybrid MSMGFSCCK method.

Figure 4 compares the nondimensional radiative heat fluxes for the case of 1 bar total pressure and a step change in temperature only as calculated by several methods. The mole fractions of the component gases are kept uniform throughout the two-layer slab. The percentage errors of the MSMGFSCCK and the single-scale FSCCK calculations compared to LBL results are also shown in the figure. In order to compare accuracy of the new database with respect to the previous one, results are obtained from both the previous MG database created by Zhang and Modest [10,16] and the newly created MG database in this paper. For a temperature inhomogeneity of this magnitude (a drop from 1500 K to 300 K), the FSCCK method gives more than 20% error as the cold layer length becomes larger than 80 cm, indicating the failure of the correlated absorption coefficient assumption. The errors of the MSMGFSCCK method while using the new MG database, on the other hand, stay below 1.6% for any cold layer thickness. The number of the groups indicated in the figure is the number of groups into which each gas scale is separated. As can be seen from Fig. 4, the accuracy of the hybrid MSMGFSCCK method is excellent, with the accuracy of the two-group case actually being better than for the four-group case, which apparently is due to the presence of compensating errors between grouping of absorption coefficients and mixing between two different absorbing gases. It has been shown by Modest and Riazzi [25] that for an isothermal layer of a gas mixture, the error incurred during heat transfer calculations is about 2% when the $k-g$ -distributions are mixed at the full-spectrum level. Hence, a MG database of combustion

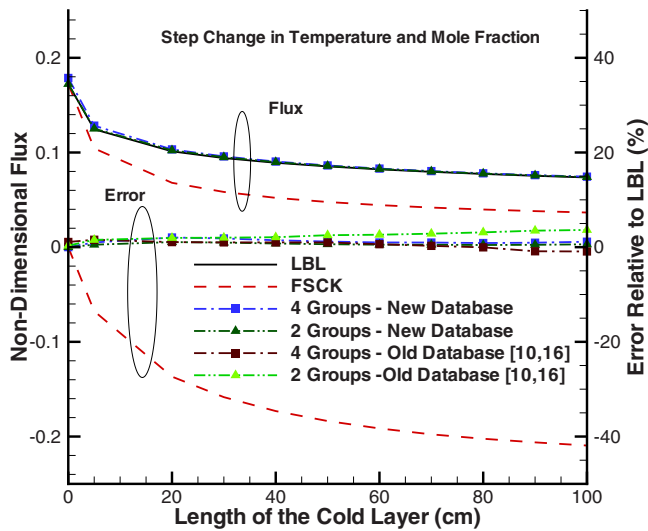


Fig. 5 Nondimensional heat flux leaving an inhomogeneous slab at a total pressure of 1 bar with step changes in temperature and mole fraction: The hot left layer contains 20% CO₂ and 10% H₂O at 1500 K and the cold right layer contains 10% CO₂ and 20% H₂O

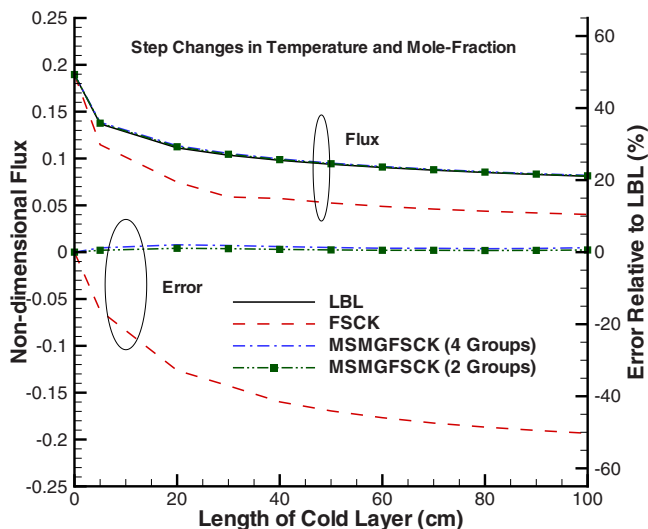


Fig. 6 Nondimensional heat flux leaving an inhomogeneous slab at a total pressure of 10 bar with step changes in temperature and mole fraction: The hot left layer contains 20% CO₂ and 10% H₂O at 1500 K and the cold right layer contains 10% CO₂ and 20% H₂O

gases with four or even two groups is sufficient to optimize between accuracy and numerical efficiency. Comparison with the data of Wang and Modest [22], in which the database created by Zhang and Modest [10,16] was used, verifies that the new MG database is superior, especially for the two-group case.

Figure 5 shows the results for a case including mole-fraction step changes in both CO₂ and H₂O in addition to a temperature step change as in Fig. 4. The left hot layer contains 20% CO₂ and 10% H₂O, and this composition is switched in the right cold layer. The total pressure of the gas mixture is 1 bar. The error of the FSK method reaches more than 40% for this extremely inhomogeneous problem. On the other hand, the four- and two-group hybrid models provide excellent results with the maximum error remaining below 2%. Results from the new database are consid-

erably more accurate than those of Wang and Modest [22] for the four-group case, and even more significantly for the two-group case.

Radiative calculations were also performed for a case of higher total gas pressure. Figure 6 shows the results for a case similar to the one in Fig. 5 except that the total gas pressure is raised to 10 bar. Again, it is observed that the MSMGFSCCK formulation in conjunction with the new MG database predicts heat transfer calculations very accurately. The errors for the four- and two-group models remain limited to within 2%, whereas the FSK methods produce more than 50% error. Hence, the results suggest that this new hybrid MSMGFSCCK model together with the MG databases can efficiently perform over a wide range of gas states.

Conclusion

In this paper, a new FSK method was developed for radiative transfer in strongly inhomogeneous gas media. The method combines the advantages of the MSFSK method in handling the mixing problem and partial pressure inhomogeneities and those of the MSFSK method in handling temperature inhomogeneities. In this method, the absorption coefficient of the mixture is broken up into contributions from the gas components, and the absorption coefficient of each component gas is subsequently separated into exclusive correlated groups. The overlap between a group and all other gases is approximately treated. As the number of groups in each gas scale increases, the effect in the approximate treatment of the overlap becomes diminished. A new MSFSK database of improved accuracy has also been constructed for the most important combustion gases, carbon dioxide and water vapor. To optimize between computational efficiency and accuracy in radiative heat transfer calculations, this MG database contains four groups for each gas species. The accuracy of the new method was established by performing sample calculations for radiative transfer in strongly inhomogeneous media using the newly constructed database. It was found that the new method successfully handles extreme inhomogeneous problems with only two or four groups for each gas component.

Acknowledgment

This research has been supported by National Science Foundation under Grant No. CTS-0121573.

Nomenclature

- a = nongray stretching factor for FSK method
- f = k -distribution function, cm
- g = cumulative k -distribution
- H = Heaviside step function
- I = radiative intensity, W/m² sr
- k = absorption coefficient variable, cm⁻¹
- k^* = overlap parameter defined in Eq. (15)
- L = geometric length, cm
- M = number of groups for a gas component
- N = number of species/scales
- P = pressure, bar
- q = radiative heat flux, W/m²
- s = distance along path, cm
- T = temperature, K
- x, \underline{x} = mole fraction (vector)

Greek Symbols

- η = wavenumber, cm⁻¹
- ϕ = composition variable vector
- δ = Dirac delta function
- λ = overlap coefficient defined in Eq. (11), cm⁻¹
- κ = absorption coefficient, cm⁻¹
- σ = Stefan-Boltzmann constant, =5.67 × 10⁻⁸ W/m² K⁴

Subscripts

- 0 = reference condition
- b = blackbody emission
- L = left layer
- l = l th gas/scale
- m = m th group
- n = n th gas/scale
- q = q th group
- R = right layer
- w = wall
- η = spectral variable in wavenumber space
- g = spectral variable in g -space

References

- [1] Lacis, A. A., and Oinas, V., 1991, "A Description of the Correlated- k Distribution Method for Modeling Nongray Gaseous Absorption, Thermal Emission, and Multiple Scattering in Vertically Inhomogeneous Atmospheres," *J. Geophys. Res.*, **96**(D5), pp. 9027–9063.
- [2] Goody, R. M., and Yung, Y. L., 1989, *Atmospheric Radiation: Theoretical Basis*, 2nd ed, Oxford University Press, New York.
- [3] Denison, M. K., and Webb, B. W., 1993, "A Spectral Line Based Weighted-Sum-of-Gray-Gases Model for Arbitrary RTE Solvers," *ASME J. Heat Transfer*, **115**, pp. 1004–1012.
- [4] Denison, M. K., and Webb, B. W., 1995, "The Spectral-Line-Based Weighted-Sum-of-Gray-Gases Model in Nonisothermal Nonhomogeneous Media," *ASME J. Heat Transfer*, **117**, pp. 359–365.
- [5] Rivière, Ph., Soufiani, A., Perrin, M. Y., Riad, H., and Gleizes, A., 1996, "Air Mixture Radiative Property Modelling in the Temperature Range 10000–40000 K," *J. Quant. Spectrosc. Radiat. Transf.*, **56**, pp. 29–45.
- [6] Pierrot, L., Rivière, Ph., Soufiani, A., and Taine, J., 1999, "A Fictitious-Gas-Based Absorption Distribution Function Global Model for Radiative Transfer in Hot Gases," *J. Quant. Spectrosc. Radiat. Transf.*, **62**, pp. 609–624.
- [7] Modest, M. F., and Zhang, H., 2002, "The Full-Spectrum Correlated- k Distribution for Thermal Radiation From Molecular Gas-Particulate Mixtures," *ASME J. Heat Transfer*, **124**(1), pp. 30–38.
- [8] Modest, M. F., 2003, "Narrow-Band and Full-Spectrum k -Distributions for Radiative Heat Transfer-Correlated- k vs. Scaling Approximation," *J. Quant. Spectrosc. Radiat. Transf.*, **76**(1), pp. 69–83.
- [9] Zhang, H., and Modest, M. F., 2002, "A Multi-Scale Full-Spectrum Correlated- k Distribution for Radiative Heat Transfer in Inhomogeneous Gas Mixtures," *J. Quant. Spectrosc. Radiat. Transf.*, **73**(2–5), pp. 349–360.
- [10] Zhang, H., and Modest, M. F., 2003, "Scalable Multi-Group Full-Spectrum Correlated- k Distributions for Radiative Heat Transfer," *ASME J. Heat Transfer*, **125**(3), pp. 454–461.
- [11] Goody, R. M., West, R., Chen, L., and Crisp, D., 1989, "The Correlated k Method for Radiation Calculations in Nonhomogeneous Atmospheres," *J. Quant. Spectrosc. Radiat. Transf.*, **42**, pp. 539–550.
- [12] Fu, Q., and Liou, K. N., 1992, "On the Correlated k -Distribution Method for Radiative Transfer in Nonhomogeneous Atmospheres," *J. Atmos. Sci.*, **49**(22), pp. 2139–2156.
- [13] Rivière, P., Soufiani, A., and Taine, J., 1992, "Correlated- k and Fictitious Gas Methods for H₂O Near 2.7 μ m," *J. Quant. Spectrosc. Radiat. Transf.*, **48**, pp. 187–203.
- [14] Rivière, P., Scutaru, D., Soufiani, A., and Taine, J., 1994, "A New c - k Data Base Suitable From 300 to 2500 K for Spectrally Correlated Radiative Transfer in CO₂-H₂O Transparent Gas Mixtures," *Tenth International Heat Transfer Conference*, Taylor & Francis, pp. 129–134.
- [15] Rivière, P., Soufiani, A., and Taine, J., 1995, "Correlated- k and Fictitious Gas Model for H₂O Infrared Radiation in the Voigt Regime," *J. Quant. Spectrosc. Radiat. Transf.*, **53**, pp. 335–346.
- [16] Zhang, H., and Modest, M. F., 2003, "Multi-Group Full-Spectrum k -Distribution Database for Water Vapor Mixtures in Radiative Transfer Calculations," *Int. J. Heat Mass Transfer*, **46**(19), pp. 3593–3603.
- [17] Wang, L., and Modest, M. F., 2005, "Narrow-Band Based Multi-Scale Full-Spectrum k -Distribution Method for Radiative Transfer in Inhomogeneous Gas Mixtures," *ASME J. Heat Transfer*, **127**, pp. 740–748.
- [18] Rothman, L. S., Barbe, A., Benner, D. C., Brown, L. R., Camy-Peyret, C., Carleer, M. R., Chance, K., Clerbaux, C., Dana, V., Devi, V. M., Fayt, A., Flaud, J.-M., Gamache, R. R., Goldman, A., Jacquemart, D., Jucks, K. W., Lafferty, W. J., Mandin, J.-Y., Massie, S. T., Nemtchinov, V., Newnham, D. A., Perrin, A., Rinsland, C. P., Schroeder, J., Smith, K. M., Smith, M. A. H., Tang, K., Toth, R. A., Vander Auwera, J., Varanasi, P., and Yoshino, K., 2003, "The HITRAN Spectroscopic Molecular Database: Edition of 2000 Including Updates Through 2001," *J. Quant. Spectrosc. Radiat. Transf.*, **82**(1–4), pp. 5–44.
- [19] Rothman, L. S., Camy-Peyret, C., Flaud, J.-M., Gamache, R. R., Goldman, A., Goorvitch, D., Hawkins, R. L., Schroeder, J., Selby, J. E. A., and Wattson, R. B., 2000, "HITEMP, the High-Temperature Molecular Spectroscopic Database," Available Through <http://www.hitran.com>.
- [20] Tashkun, S. A., Perevalov, V. I., Bykov, A. D., Lavrentieva, N. N., and Teffo, J.-L., 2002, "Carbon Dioxide Spectroscopic Databank (CDSD)," Available From <ftp://ftp.iao.ru/pub/CDSD-1000>.
- [21] Modest, M. F., and Bharadwaj, S. P., 2002, "High-Resolution, High-Temperature Transmissivity Measurements and Correlations for Carbon Dioxide-Nitrogen Mixtures," *J. Quant. Spectrosc. Radiat. Transf.*, **73**(2–5), pp. 329–338.
- [22] Wang, L., and Modest, M. F., 2005, "A Hybrid Multi-Scale Full-Spectrum k -Distribution Method for Radiative Transfer in Inhomogeneous Gas Mixtures," *Proceedings of IMECE 2005*, Orlando, FL, ASME.
- [23] Modest, M. F., 2003, *Radiative Heat Transfer*, 2nd ed., Academic, New York.
- [24] Wang, A., and Modest, M. F., 2007, "An Adaptive Emission Model for Monte Carlo Ray-Tracing in Participating Media Represented by Statistical Particle Fields," *J. Quant. Spectrosc. Radiat. Transf.*, **104**(2), pp. 288–296.
- [25] Modest, M. F., and Riazzi, R. J., 2004, "Assembly of Full-Spectrum k -Distributions From a Narrow-Band Database; Effects of Mixing Gases, Gases and Nongray Absorbing Particles, and Mixtures With Nongray Scatterers in Nongray Enclosures," *J. Quant. Spectrosc. Radiat. Transf.*, **90**(2), pp. 169–189.
- [26] Wang, A., and Modest, M. F., 2005, "High-Accuracy, Compact Database of Narrow-Band k -Distributions for Water Vapor and Carbon Dioxide," *J. Quant. Spectrosc. Radiat. Transf.*, **93**, pp. 245–261.