

DRAFT

IMECE2005-82642

A HYBRID MULTI-SCALE FULL-SPECTRUM k -DISTRIBUTION METHOD FOR RADIATIVE TRANSFER IN INHOMOGENEOUS GAS MIXTURES

Liangyu Wang

Department of Mechanical and Nuclear Engineering
The Pennsylvania State University
University park, PA 16802
Email: lxw192@psu.edu

Michael F. Modest*

Department of Mechanical and Nuclear Engineering
The Pennsylvania State University
University park, PA 16802
Email: mfmodest@psu.edu

ABSTRACT

A new full-spectrum k -distribution (FSK) method has been developed, which integrates the advantage of the multi-group FSK method in dealing with temperature inhomogeneities for single-species media with the advantages of the multi-scale FSK method in dealing with partial pressure inhomogeneities for gas mixtures. The new method can achieve great accuracy for radiative heat transfer calculations in participating media with inhomogeneities in both temperature and gas concentrations. The mathematical development of the new method is described, and several sample calculations are performed to demonstrate the accuracy of the new method by comparison with line-by-line calculations.

Keywords: k-Distribution Method, Inhomogeneous Gas Mixture, Multi-Scale Approach, Multi-Group Approach

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/m ² 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/m ²
Q	quantity defined in Eq. (23)
s	distance along path, cm
T	temperature, K
x, \underline{x}	mole fraction (vector)
\mathcal{L}	Laplace transform

Greek Symbols

η	wavenumber, cm ⁻¹
$\underline{\phi}$	composition variable vector
δ	Dirac's delta function
λ	overlap coefficient defined in Eq. (11), cm ⁻¹
κ	absorption coefficient, cm ⁻¹
σ	Stefan-Boltzmann constant

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 in wavenumber space
g	spectral in g space

*Address all correspondence to this author.

Introduction

Radiative transfer calculations in participating media are hindered by the irregular gas-phase absorption coefficients that seem to vary randomly across the spectrum. In general, spectral integration of radiative quantities must invoke the line-by-line (LBL) approach for satisfactory accuracy. This comes at the expense of heavy computational time since millions of evaluations of the radiative transfer equation (RTE) are involved. On the other hand, the absorption coefficient can be reordered statistically [1, 2], such that only ten or fewer quadrature point evaluations of the RTE are required. This greatly reduces the computational cost, but at the expense of accuracy for highly inhomogeneous media. Examples of such reordering processes include the spectral-line-based weighed-sum-gray-gases (SLW) model [3, 4], the absorption distribution function (ADF) method [5, 6], and the full-spectrum k -distribution (FSK) method [7]. The FSK method, with several major developments [8–13], has become the most promising spectral model for radiative transfer in participating media.

Challenges remains, however, in applying the FSK method, or any other global methods, to strongly inhomogeneous emitting and absorbing mixtures. Inhomogeneities in total pressure, temperature, and component gas mole fraction (partial pressure) change the spectral behavior of the absorption coefficient, which is critical to the FSK reordering process. The effect of varying total pressure on the FSK reordering process is relatively small, as evidenced by the success of applying the correlated- k method in the field of meteorology, where strong total pressure variations occur while temperatures stay relatively uniform [1, 14, 15]. The effects of varying temperature and varying gas concentrations can be substantial, as recognized by Rivière et al. [16–18] and by Modest and Zhang [7].

The inhomogeneity problem can be addressed by several strategies with different levels of sophistication and accuracy. Commonly used strategies include the correlated absorption coefficient assumption and the scaling approximation. The correlated assumption requires that the maximum and minimum absorption coefficients across the spectrum always occur at the same wavenumber. The scaling approximation, a special case of a correlated absorption coefficient, is somewhat more restrictive, and requires that spectral and spatial dependence of the absorption coefficient be separable. The subtle differences between the two approaches have been elucidated by Modest [8]. The SLW model and the ADF method use the correlated approach for inhomogeneous media. The application of both the correlated and the scaled approaches to the FSK method leads to the full-spectrum correlated k -distribution (FSCK) and scaled k -distribution (FSSK) methods [8].

The correlated and scaled methods can produce accurate results for media that have large variations in total pressure but small variations in temperature and partial pressure. For media that have large temperature and partial pressure variations,

the errors introduced by the two methods can be substantial. Another strategy of dealing with inhomogeneity problems is to break up gas absorption coefficients into pieces that are as correlated or scaled as possible. There have been two approaches to implement this strategy, the fictitious gases (FG) [6] and the multi-group (MG) [10, 19] approach. In the fictitious gas approach the individual spectral lines comprising the absorption coefficient are placed into separate groups based on their temperature dependence. Examples of this implementation include the fictitious-gas-based ADF (ADFFG) method [6] and the multi-scale FSK (MSFSK) method [9]. In the multi-group approach, on the other hand, spectral positions (e.g., wavenumbers) are placed into spectral groups according to their dependence on temperature and partial pressure. Databases for the multi-group FSK (MGFSK) method have been constructed for CO₂ and H₂O [10, 19]. Both approaches, with increased correlatedness within each fictitious gas and spectral group, improve the accuracy of radiation calculations in inhomogeneous problems.

The multi-group approach, however, has the advantage of computational efficiency over the fictitious gas approach. If the number of fictitious gases or spectral groups is M , then the fictitious gas approach needs to solve M^2 independent RTE's, while the multi-group approach needs to solve only M , since there is no overlap among different spectral groups. Note that the multi-scale FSK method, when taking the fictitious gas approach, avoids the extra computational cost problem by introducing an approximate overlap parameter and, therefore, also requires only M RTE solutions [9, 12], although at a slight loss of accuracy.

The MGFSK method has been shown to be able to achieve great accuracy and computational efficiency for single species inhomogeneous gases [10, 19]. For inhomogeneous mixtures, however, spectral groups from different gas species are incompatible, and it appears impossible to obtain k -distributions for arbitrary gas mixtures from mixing those of individual species. On the other hand, the MSFSK method can treat, in addition to the fictitious gases, the absorption coefficient of an individual species in a mixture as one of its scales. It solves the mixing problem by introducing an overlap coefficient to resolve the overlap among scales [12].

It is the purpose of the present paper to develop a new hybrid FSK scheme that combines the advantages of the MSFSK and MGFSK methods and is capable of handling radiative transfer in inhomogeneous mixtures with great accuracy and computational efficiency. The mathematical development for the new scheme is described in detail. Sample calculations are performed for a mixture with extreme inhomogeneities in gas concentration and temperature, and the results are compared to LBL calculations.

The Hybrid Multi-Scale/Group Approach

Although the following development can be easily extended to include gray absorbing and scattering particles, for clarity, a

medium consisting of a mixture of molecular gases is considered, and the radiative transfer equation (RTE) is then written as [20]

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

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 the absorption coefficient, $I_{b\eta}$ the spectral blackbody intensity (or Planck function), and wave number 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 the emission and/or reflection from the enclosure wall [21].

The total absorption coefficient κ_η is first separated into contributions from the N component gases, e.g., CO_2 and H_2O , and then the spectral locations of the n -th gas absorption coefficient are sorted into M exclusive spectral groups, i.e.,

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

where the radiative intensity I_η is broken up accordingly. 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 RTE's, one for each group of each gas or scale:

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

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 from all groups of other gases plus its own group. There is no overlap among groups within each gas scale, that is, for 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 [8] to the RTE of each group: first Eq. (4) is multiplied by Dirac's delta function $\delta(k_{nm} - \kappa_{nm\eta}(\underline{\phi}))$, followed by division with

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

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

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

where

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

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

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

$$\lambda_{nm} I_{nmg} = k_{nm} I_{nmg} + \frac{\int_0^\infty \left(\sum_{l \neq n} \sum_{q=1}^{M_l} \kappa_{lq\eta}(\underline{\phi}) \right) I_{nm\eta} \delta(k_{nm} - \kappa_{nm\eta}(\underline{\phi}_0)) d\eta}{f_{nm}(T_0, \underline{\phi}_0, k_{nm})}. \quad (11)$$

Here the absorption coefficient within each group has been assumed to be correlated. This implies that $k_{nm} = k_{nm}(T_0, \underline{\phi}, g_{nm})$ 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 [8]. The error due to the correlated assumption, however, is greatly reduced or even eliminated since the groups are established such that the absorption coefficient of each group satisfies the correlated assumption or the scaled approximation. Zhang and Modest [10, 19] have constructed two such 32-group databases for CO_2 and H_2O , according to the temperature and partial pressure dependencies of the absorption coefficients. The absorption coefficients at the 32 group level satisfy the scaled approximation to a great degree of accuracy and LBL accuracy can be obtained for inhomogeneous radiation calculations with a number of groups often even less than 32. The databases are scalable, that is, for greater numerical efficiency (accompanied by a slight loss of accuracy), the spectral groups from the databases can be combined to obtain a coarser number of groups. These 32-group databases are utilized here to construct the $k-g$ distributions and the nongray stretching functions

a required in Eq. (7) (the k_{nm} and the a_{nm} terms). The combination of groups and the evaluation of a functions are detailed in [10, 19].

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 determined approximately 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.

In Eq. (7), the reordering is performed in terms of $\kappa_{nm\eta}$ and the overlap 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

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

where

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

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

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

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 obtained analytically, and the total exiting intensities at $s = L$ are

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

and

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

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

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

or

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

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 using the relationship [9]

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

In wavenumber space this may 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 equation for the λ_{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 equation 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 32-group databases. The right hand side (RHS) of Eq. (20) contains the k_{nm}^* term, which may be calculated directly from Eq. (15) using high-resolution spectral 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 be able to evaluate the RHS of Eq. (15) using the same multi-group databases.

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

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

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

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

where $\kappa_{l\eta}$ is the total (or single group) absorption coefficient of the l -th gas/species. The second step follows by recognizing that the integration 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 32-group databases are full-spectrum k -distributions, the mixing in Eq. (25) is at a full-spectrum level and, thus, is expected to be somewhat less accurate than on a narrow band level [11]. However, the uncorrelated assumption should be reasonable here since the nm -th group not only comes from a different gas *but also* it consists of scattered parts of the spectrum.

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

which is rewritten as

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

Here $k_l - g_l$ is the k - g distribution of the entire l -th gas, and can be obtained from the multi-group database by combining all 32 groups into one [19],

$$g_l(T, \underline{\phi}, k_l) = \sum_{q=1}^{32} g_{lq}(T, \underline{\phi}, k_{lq}) - 31, \quad (27)$$

evaluated at any given $k_l = k_{lq}$.

Equating Eqs. (26) and (24) gives,

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

and the integral property of the Laplace transform gives,

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

Finally, taking the inverse Laplace transform gives

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

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

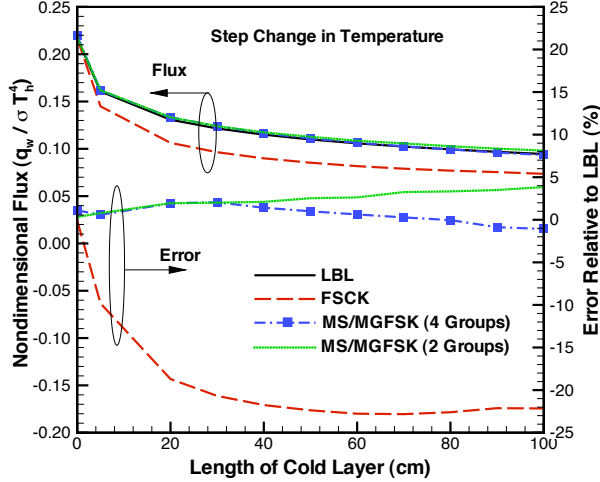


Figure 1. **Nondimensional heat flux leaving an inhomogeneous slab of 10% CO₂ and 20% H₂O with a step change in temperature: the hot left layer is at 1500 K and the cold right layer 300 K.**

on group k -distributions constructed from the multi-group databases:

$$\int_0^{g_{nm}(k_{nm})} k'_{nm} dg'_{nm} = \int_{g_{nm}=0}^1 \prod_{l \neq n} \left(\int_{g_l=0}^1 k_{nm} \times H(\lambda_{nm} - \sum_{l \neq n} k_l - k_{nm}) dg_l \right) dg_{nm}, \quad (31)$$

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

For special cases, for example, for a mixture of two gases, the λ_{1m} - k_{1m} relation for the m -th group of gas 1 can be found from

$$\int_0^{g_{1m}(k_{1m})} k'_{1m} dg'_{1m} = \int_{g_{1m}=0}^1 k_{1m} g_2 (\lambda_{1m} - k_{1m}) dg_{1m}, \quad (32)$$

and similarly for other groups in gas 1 and 2.

Sample Calculations

To illustrate the performance of the new method in handling inhomogeneous problems, a few sample calculations with extreme temperature and mole fraction (partial pressure) inhomogeneities are carried out. In all cases, a mixture of CO₂-H₂O-N₂ confined between cold black walls is considered. The mixture is

at a total pressure of 1 bar and consists of two different homogeneous layers (denoted as left and right layer/column) adjacent to each other. The left layer is at 1500 K and has a fixed width of 50 cm. The right layer is cold at 300 K and the length of this layer is varied in the calculations. The radiative heat flux leaving from the right layer is calculated using the LBL method, the (single scale) full-spectrum correlated- k (FSCK) method, and the hybrid multi-scale/group FSK method.

For consistency, the HITEMP [22] spectral database is used to calculate the absorption coefficients of both H₂O and CO₂, since the 32-group databases [10, 19] for H₂O and CO₂ were constructed from the HITEMP database. In the hybrid FSK calculations the required k - g distributions (in the RTE evaluations and the determination of the overlap coefficients) are constructed from the 32-group databases, while in the single scale FSCK calculations the required k - g distributions are obtained directly from the absorption coefficients computed from the HITEMP database, and there is no mixing involved, i.e., the absorption coefficients are calculated for the entire mixture. The LBL calculations serve as benchmark and the FSCK calculations serve as demonstration of the improvement made by the hybrid FSK method.

Figure 1 shows the calculated nondimensional radiative heat fluxes for the case of a severe step change in temperature only. The mole fractions of the component gases are kept uniform throughout the two-layer slab. The percentage errors of the hybrid FSK and the single scale FSCK calculations compared to LBL results are also shown in the figure. In both the hybrid and single scale FSCK calculations, a Gaussian quadrature scheme is used consistently and 10 quadrature points and weights are selected. For the temperature inhomogeneity of this magnitude (a drop from 1500 K to 300 K), the FSCK method gives more than 20% errors as the cold layer length becomes larger than 20 cm, indicating failure of the correlated absorption coefficient assumption. The errors of the hybrid FSK method, on the other hand, stay below 5% for the different cold layer lengths.

The number of groups indicated in the figure is the number of groups separated in each gas/scale. As can be seen in the figure, the higher the number of groups, the more accurate the hybrid method, since increasing the number of groups in each scale improves the correlatedness assumption within each group. It may also increase the uncorrelatedness between groups and gas scales, as required for mixing in Eq. (25). However, increasing the number of groups increases the computational cost since more RTE's need to be evaluated. Here only two and four groups are considered, and both two and four group models give satisfactory results for this severe case. Note that the same number of groups is used for different gases/scales in the calculations, the use of different numbers of groups may improve computational efficiency without degrading the accuracy. However, for more realistic applications (i.e., no abrupt step changes in temperature or concentration), the use of more than two groups will probably

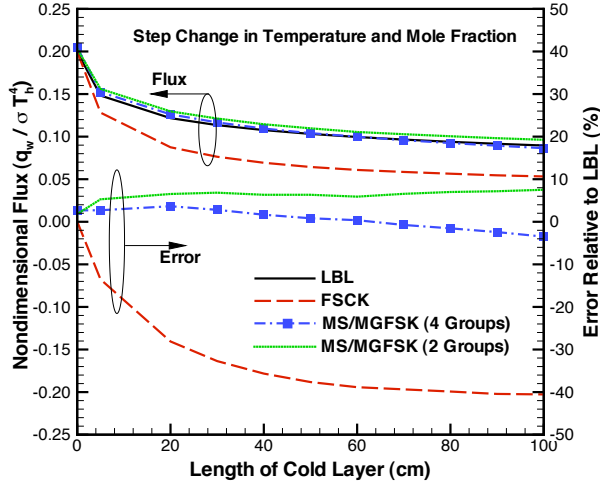


Figure 2. Nondimensional heat flux leaving an inhomogeneous slab with step changes in temperature and mole fractions: the hot left layer contains 20% CO₂ and 10% H₂O at 1500 K and the cold layer contains 10% CO₂ and 20% H₂O at 300 K.

rarely be warranted.

Figure 2 shows the results for a case including mole fraction step changes in both H₂O and CO₂ in addition to a temperature step change. The left hot layer contains 20% CO₂ and 10% H₂O, and this composition is switched in the right cold layer. The error of the FSCK method reaches more than 40% for this extremely inhomogeneous problem. On the other hand, the four group hybrid model still gives satisfactory results, although the two group model becomes somewhat inaccurate for large cold layer lengths. However, given the extreme nature of this problem, the error introduced by the two group hybrid model can be considered to be acceptable.

The composition used in Fig. 2 is switched (i.e., 10% CO₂ and 20% H₂O in the left hot layer and 20% CO₂ and 10% H₂O in the cold layer) and the results are shown in Fig. 3. Compared to the case in Fig. 1, the absorption in the cold layer due to CO₂ is doubled, while the absorption due to H₂O is halved. The error from the FSCK method is now on the level of about 13% since H₂O emission is dominant and it occurs almost everywhere across the spectrum. The error introduced by the new hybrid method stays below 3% with the 4 group model achieves slightly more accurate results. This shows that the new FSK method performs consistently well in different cases and the two group hybrid model is able to achieve satisfactory results compared to LBL calculations.

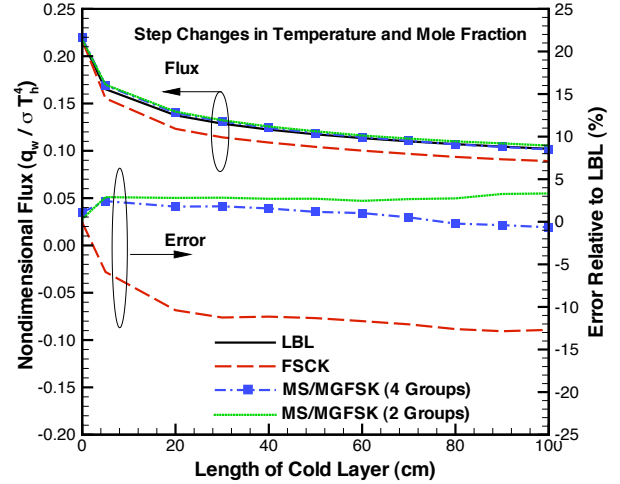


Figure 3. Nondimensional heat flux leaving an inhomogeneous slab with step changes in temperature and mole fractions: the hot left layer contains 10% CO₂ and 20% H₂O at 1500 K and the cold layer contains 20% CO₂ and 10% H₂O at 300 K.

Summary and Conclusions

In this paper a new full-spectrum *k*-distribution method was developed for radiative transfer in strongly inhomogeneous gas media. The method combines the advantages of the multi-scale full-spectrum *k*-distribution method in handling the mixing problem and partial pressure inhomogeneities, and those of the multi-group full-spectrum *k*-distribution 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 treated approximately. As the number of groups in each gas scale increases, the effect in the approximate treatment of the overlap becomes diminished. The accuracy of the new method was established by performing sample calculations for radiative transfer in strongly inhomogeneous media. It was found that the new method successfully handles extreme inhomogeneous problems with only two or four groups for each gas component.

Acknowledgments

This research has been sponsored by National Science Foundation under Grant Number CTS-0112423 and CTS-0121573.

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", *Journal of Geophysical Research*, **96**(D5), pp. 9027–9063.
- [2] Goody, R. M. and Yung, Y. L., 1989, *Atmospheric Radiation – Theoretical Basis*, Oxford University Press, New York, 2nd ed.
- [3] Denison, M. K. and Webb, B. W., 1993, "A Spectral Line Based Weighted-Sum-of-Gray-gases Model for Arbitrary RTE Solvers", *ASME Journal of 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 Non-isothermal Nonhomogeneous Media", *ASME Journal of 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", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **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", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **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 Journal of 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", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **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", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **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 Journal of Heat Transfer*, **125**(3), pp. 454–461.
- [11] 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", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **90**(2), pp. 169–189.
- [12] 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 Journal of Heat Transfer*, in print.
- [13] Wang, L. and Modest, M. F., 2005, "Treatment of Wall Emission in the Narrow-Band Based Multi-Scale Full-Spectrum k -Distribution Method", *ASME Journal of Heat Transfer*, **127**, submitted for publication.
- [14] Goody, R. M., West, R., Chen, L., and Crisp, D., 1989, "The Correlated k Method for Radiation Calculations in Nonhomogeneous Atmospheres", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **42**, pp. 539–550.
- [15] Fu, Q. and Liou, K. N., 1992, "On the Correlated k -Distribution Method for Radiative Transfer in Nonhomogeneous Atmospheres", *Journal of the Atmospheric Sciences*, **49**(22), pp. 2139–2156.
- [16] Rivière, P., Soufiani, A., and Taine, J., 1992, "Correlated- k and Fictitious Gas Methods for H₂O near 2.7 μ m", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **48**, pp. 187–203.
- [17] 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", In *Tenth International Heat Transfer Conference*, Taylor & Francis, pp. 129–134.
- [18] Rivière, P., Soufiani, A., and Taine, J., 1995, "Correlated- k and Fictitious Gas Model for H₂O Infrared Radiation in the Voigt Regime", *Journal of Quantitative Spectroscopy and Radiative Transfer*, **53**, pp. 335–346.
- [19] Zhang, H. and Modest, M. F., 2003, "Multi-Group Full-Spectrum k -Distribution Database For Water Vapor Mixtures in Radiative Transfer Calculations", *International Journal of Heat and Mass Transfer*, **46**(19), pp. 3593–3603.
- [20] Modest, M. F., 2003, *Radiative Heat Transfer*, Academic Press, New York, 2nd ed.
- [21] Wang, L. and Modest, M. F., 2005, "Multi-Scale Full-Spectrum k -Distribution Method for Radiative Transfer in Inhomogeneous Gas Mixtures with Wall Emission", In Webb and Modest?, eds., *Proceedings of the 2005 ASME Summer Heat Transfer Conference*, San Francisco, CA.
- [22] 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>.