

Treatment of Wall Emission in the Narrow-Band Based Multiscale Full-Spectrum k -Distribution Method

Liangyu Wang

Michael F. Modest¹

Fellow ASME
e-mail: MFModest@psu.edu

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

The multiscale full-spectrum k -distribution (MSFSK) method has become a promising method for radiative heat transfer in inhomogeneous media. In this paper a new scheme is proposed to extend the MSFSK's ability in dealing with boundary wall emission by distributing this emission across the different gas scales. This scheme pursues the overlap concept of the MSFSK method and requires no changes in the original MSFSK formulation. A boundary emission distribution function is introduced and two approaches of evaluating the function are outlined. The first approach involves line-by-line integration of the spectral absorption coefficients and is, therefore, impractical. The second approach employs a narrow-band k -distribution database to calculate all parameters as in the original narrow-banded based MSFSK formulation and is, therefore, efficient. This distribution scheme of wall emission is evaluated and the two approaches are compared by conducting sample calculations for radiative heat transfer in strongly inhomogeneous media using both the MSFSK method and the line-by-line method.

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Introduction

Because of the strongly irregular spectral variations of gas absorption coefficients, high spectral resolution calculations (often referred to as line-by-line, LBL, approach) have to be generally invoked to accurately predict radiative heat transfer in participating media. LBL calculations require millions of evaluations of the radiative transfer equation (RTE) and, therefore, consume an enormous computational effort. On the other hand, the k -distribution method [1,2] reorders the absorption coefficients into monotonic k -distributions and, thus, greatly reduces the computational cost by using only ten or fewer quadrature evaluations of the RTE. The development of the full-spectrum k -distribution method (FSK) [3] further facilitates the application of the method to practical problems.

Challenges remain, however, in applying the FSK method to inhomogeneous emitting and absorbing mixtures. Inhomogeneities in total pressure, temperature, and component gas mole fraction (partial pressure) change the spectral distribution 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 [1,4,5]. The effects of varying temperature and varying gas concentrations can be substantial, as recognized by Rivière et al. [6–8] and by Modest and Zhang [3]. They are the focus of further FSK developments.

The multigroup FSK (MGFSK) [9] and multiscale FSK (MSFSK) [10] have been developed to deal with the temperature and partial pressure inhomogeneities. The MGFSK method arranges

spectral positions into M separate groups according to their temperature and partial pressure dependencies. There is no overlap among different groups and, therefore, the method requires only $M \times N$ (N being the number of quadrature points) RTE evaluations without any further approximation. Although the MGFSK method can achieve great accuracy for individual gases, groups from different gases are incompatible and it appears impossible to apply the MGFSK method to problems involving inhomogeneous mixtures.

The MSFSK method, on the other hand, groups individual spectral lines comprising the absorption coefficient into M separate scales according to their temperature dependence: The overlap in spectrum between different scales is treated in an approximate way so that $M \times N$ RTE evaluations are required. The MSFSK method can also treat the absorption coefficient of an individual species in a mixture as one of its scales. It has been found that in addition to eliminating the error caused by partial pressure (gas concentration) inhomogeneities, breaking up a gas mixture into gas scales reduces the error caused by temperature inhomogeneities [11]. The multiscale approach is therefore preferred in the treatment of mixture inhomogeneities with the FSK method.

One of the essential features of the MSFSK method is the overlap coefficient λ , and this coefficient is determined such that the radiative transfer in a homogeneous medium is predicted exactly using the MSFSK scheme. At the present state of development, however, the MSFSK method, unlike the single scale FSK method [3], and the spectral-line-based weighted-sum-gray-gases method [12,13], is limited to media surrounded by cold, nonemitting walls. It is desirable to include wall emission in the general MSFSK formulation, so that the method can also handle situations in which wall emission plays an important role in the radiative heat transfer.

It is the purpose of this paper to introduce an effective scheme to account for gray wall emission in the MSFSK method. The scheme pursues the concept of the overlap coefficient and keeps

¹Corresponding author.

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the original MSFSK formulation unchanged. A boundary emission distribution function is introduced. To keep the method as practical as the original narrow-band based MSFSK method, a formula is derived that employs the same database of narrow-band k -distributions to calculate the distribution function. The mathematical development for the boundary scheme is described, followed by validation of the approach. Sample calculations are performed for a mixture with extreme inhomogeneities in gas concentration and temperature, and the results are compared with LBL calculations.

Theoretical Development

MSFSK Formulation With Boundary Emission. Although the following development can easily be extended to include gray absorbing and scattering particles, for clarity a medium consisting of a mixture of molecular gases is considered, and the RTE is then written as [14]

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

subject to the boundary condition

$$\text{at } s=0: \quad I_\eta = \epsilon I_{b\eta} + \frac{1-\epsilon}{\pi} \int_{2\pi} I_\eta |\hat{n} \cdot \hat{s}| d\Omega \quad (2)$$

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 vector $\boldsymbol{\phi}$ contains state variables that affect κ_η which include temperature T , total pressure P , and gas mole fractions \mathbf{x} : $\boldsymbol{\phi}=(T, P, \mathbf{x})$. The boundary wall has been assumed to be gray with ϵ being the emittance, \hat{n} the surface normal, \hat{s} the unit direction vector of incoming ray radiation, and Ω the solid angle. If one separates the contributions to κ_η from the M component gases and breaks up the radiative intensity I_η accordingly, i.e.,

$$\kappa_\eta = \sum_{m=1}^M \kappa_{m\eta} \quad I_\eta = \sum_{m=1}^M I_{m\eta} \quad (3)$$

then the RTE (1) is transformed into M component RTEs, one for each gas or scale. In this paper, we will deal only with the treatment of concentration inhomogeneities, i.e., each gas species will be treated as a single scale. Temperature inhomogeneities will be addressed in a follow-up paper. Then the RTE for each gas scale is

$$\frac{dI_{m\eta}}{ds} = \kappa_{m\eta}(\boldsymbol{\phi})I_{b\eta} - \kappa_\eta(\boldsymbol{\phi})I_{m\eta} \quad \text{for } m=1, \dots, M \quad (4)$$

It is observed that, physically, the intensity $I_{m\eta}$ for the m th scale is due to emission from the m th gas species but subject to absorption from all gases.

It is important to note that in Eq. (4), if there is no wall emission, the spectral locations where κ_η contributes to the absorption of $I_{m\eta}$ (i.e., absorption by all the scales) are only those wave numbers for which $\kappa_{m\eta}$ is nonzero. Therefore, the overlap region is only a subset of those wave numbers with $\kappa_{m\eta} \neq 0$, across which absorption from other gases occurs as well. The original MSFSK formulation takes advantage of the fact that the overlap regions for each scale are relatively small compared to the total emission/absorption spectrum of each scale, and the fact that the absorption coefficients in the overlap regions are mostly small. If there is wall emission, however, absorption by other than the emitting scale will take place not just over the small overlap regions but across the entire spectrum. Therefore, the underlying justification of the MSFSK scheme to treat the absorption by other scales in the overlap region in an approximate fashion is no longer valid, and large errors may occur.

There are several strategies to deal with wall emission. For example, an additional scale could be used, but this would require

N additional RTE evaluations, and would complicate the accurate evaluation of an appropriate overlap coefficient. Here we propose a strategy consistent with the logic of the MSFSK method and requiring no additional computational cost: Wall emission is distributed across all scales according to the absorption coefficient of each scale, that is,

$$\text{at } s=0: \quad I_{m\eta} = \frac{\kappa_{m\eta}(\boldsymbol{\phi}_0)}{\kappa_\eta(\boldsymbol{\phi}_0)} \epsilon I_{b\eta} + \frac{1-\epsilon}{\pi} \int_{2\pi} I_{m\eta} |\hat{n} \cdot \hat{s}| d\Omega \quad (5)$$

where $\boldsymbol{\phi}_0$ denotes the reference state of the mixture. Note that the sum of Eq. (5) over all the scales reduces to Eq. (2). With such distribution, wall emission exists within each scale only at the spectral locations where medium emission takes place, and, therefore, the overlap approximation of the MSFSK method remains valid.

The overlap coefficient in the MSFSK formulation is determined by considering a homogeneous medium without wall emission. Additional considerations are required to include wall emission. We now apply the FSK scheme [15] to the RTE of each scale: First, Eq. (4) is multiplied by Dirac's delta function $\delta(k_m - \kappa_{m\eta}(\boldsymbol{\phi}_0))$, followed by division with the k -distribution of the m th scale, or

$$f_m(T_0, \boldsymbol{\phi}_0, k_m) = \frac{1}{I_b(T_0)} \int_0^\infty I_{b\eta}(T_0) \delta(k_m - \kappa_{m\eta}(\boldsymbol{\phi}_0)) d\eta \quad (6)$$

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

$$\frac{dI_{mg}}{ds} = k_m(T_0, \boldsymbol{\phi}, g_m) a_m I_b - \lambda_m I_{mg} \quad \text{for } m=1, \dots, M \quad (7)$$

where

$$I_{mg} = \int_0^\infty I_{m\eta} \delta(k_m - \kappa_{m\eta}(\boldsymbol{\phi}_0)) d\eta / f_m(T_0, \boldsymbol{\phi}_0, k_m) \quad (8)$$

$$g_m = \int_0^{k_m} f_m(T_0, \boldsymbol{\phi}_0, k) dk \quad (9)$$

$$a_m = \frac{f_m(T, \boldsymbol{\phi}_0, k_m)}{f_m(T_0, \boldsymbol{\phi}_0, k_m)} \quad (10)$$

$$\lambda_m I_{mg} = k_m(T_0, \boldsymbol{\phi}, g_m) I_{mg} + \int_0^\infty \left(\sum_{n \neq m} \kappa_{n\eta}(\boldsymbol{\phi}) \right) I_{m\eta} \times \delta(k_m - \kappa_{m\eta}(\boldsymbol{\phi}_0)) d\eta / f_m(T_0, \boldsymbol{\phi}_0, k_m) \quad (11)$$

Here the correlated- k (FSCK) approach has been taken and $k_m(T_0, \boldsymbol{\phi}, g_m)$ is the k -distribution of the absorption coefficient for the m th scale at state $\boldsymbol{\phi}$ using T_0 as the Planck function temperature [15]. Equation (11) defines the overlap coefficient, λ_m , which represents the overlap of the absorption coefficient of the m th scale, $\kappa_{m\eta}$, with those of all other scales. Overlap occurs only over a small part of the spectrum, and the overlap coefficients λ_m are in effect reordered absorption coefficients of the m th scale taking into account the overlap with all other scales. In the MSFSK approach, the λ_m are determined approximately, based on the argument that overlap effects between scales (individual gas species in this work) are relatively small.

Applying the same reordering procedure to the boundary condition (Eq. (5)), one obtains the reordered condition corresponding to Eq. (7):

$$\text{at } s=0: \quad I_{mg} = \mu_m \epsilon I_{bw} + \frac{1-\epsilon}{\pi} \int_{2\pi} I_{mg} |\hat{n} \cdot \hat{s}| d\Omega \quad (12)$$

where

$$\mu_m = \frac{1}{I_{bw}} \int_0^\infty \frac{\kappa_{m\eta}(\phi_0)}{\kappa_\eta(\phi_0)} I_{b\eta} \delta(k_m - \kappa_{m\eta}(\phi_0)) d\eta / f_m(T_0, \phi_0, k_m) \quad (13)$$

$$\int_0^{k_m} k'_m f_m(T, \phi, k'_m) dk'_m = \int_0^{k'=\lambda_m} k_m^*(k') dk' \quad (22)$$

Here μ_m is the boundary emission distribution function and can be evaluated from Eq. (13) without approximation.

Following the approach in the MSFSK method to determine the overlap coefficient, we consider the radiative intensity within a semi-infinite homogeneous gas mixture. To be consistent with the evaluation of λ_m for medium emission, the medium is assumed bounded by a black wall at a different temperature than that of the medium. The analytical solution to Eq. (7) for a homogeneous mixture bounded by a black wall may be written as

$$I_m = \int_0^1 I_{mg} dg = \int_0^\infty \mu_m I_{bw} \exp(-\lambda_m s) f_m(T, \phi, k_m) dk_m + \int_0^\infty \frac{k_m}{\lambda_m} I_b [1 - \exp(-\lambda_m s)] f_m(T, \phi, k_m) dk_m = I_{m1} + I_{m2} \quad (14)$$

where I_{m1} is short-hand for the first term (wall emission) in the second step, and I_{m2} for the second term (medium emission); the mixture temperature is T and the wall temperature is T_w .

The reordering of Eq. (4) can also be performed in terms of κ_η which, for a homogeneous layer at temperature T , leads to

$$\frac{dI_{mg}^*}{ds} = \frac{k_m^*(T) I_b}{f(T, \phi, k)} - k I_{mg}^* \quad \text{for } m = 1, \dots, M \quad (15)$$

and the corresponding boundary condition,

$$\text{at } s = 0: \quad I_{mg}^* = \frac{k_m^*(T_w)}{k} I_{bw} / f(T, \phi, k) + \frac{1 - \epsilon}{\pi} \int_{2\pi} I_{mg}^* |\hat{n} \cdot \hat{s}| d\Omega \quad (16)$$

where

$$f(T, \phi, k) = \frac{1}{I_b(T)} \int_0^\infty I_{b\eta}(T) \delta(k - \kappa_\eta(\phi)) d\eta \quad (17)$$

$$I_{mg}^* = \int_0^\infty I_{m\eta} \delta(k - \kappa_\eta(\phi)) d\eta / f(T, \phi, k) \quad (18)$$

$$k_m^*(T) = \frac{1}{I_b(T)} \int_0^\infty I_{b\eta}(T) \kappa_{m\eta} \delta(k - \kappa_\eta(\phi)) d\eta \quad (19)$$

The analytical solution to Eq. (15) for a homogeneous mixture bounded by a black wall is then written as

$$I_m^* = \int_0^1 I_{mg}^* dg = \int_0^\infty \frac{k_m^*(T_w)}{k} I_{bw} \exp(-ks) dk + \int_0^\infty \frac{k_m}{k} I_b [1 - \exp(-ks)] dk = I_{m1}^* + I_{m2}^* \quad (20)$$

where again I_{m1}^* abbreviates the first term (wall emission) in the second step, and I_{m2}^* the second term (medium emission).

The spectrally integrated intensity, I_m , must be equal to I_m^* . In the original MSFSK formulation there is no wall emission, and equating I_{m2} and I_{m2}^* leads to the determination of the overlap coefficient as [10,11]

$$\lambda_m = k \quad k_m f_m(T, \phi, k_m) dk_m = k_m^*(k) dk \quad (21)$$

The overlap coefficient is then found implicitly from [10,11]

In the presence of wall emission, I_{m1} may, in general, not be equal to I_{m1}^* if λ_m is determined from Eq. (22), since the equation is derived from considering medium emission only. In addition, the evaluation of μ_m from Eq. (13) appears to be inconvenient. We can, however, modify the definition for μ_m , Eq. (13), such that I_{m1} equals I_{m1}^* and, therefore, total intensity I_m equals I_m^* for the homogeneous case with a wall temperature different from the medium temperature. Furthermore, the modified expression for μ_m can be evaluated easily, as shown in the following.

To equate I_{m1} and I_{m1}^* , the expression for I_{m1}^* is rearranged employing the approximation of λ_m , Eq. (21):

$$I_{m1}^* = \int_0^\infty \frac{k_m^*(T_w, k) k_m^*(T, k)}{k_m^*(T, k) k} I_{bw} \exp(-ks) dk = \int_0^\infty \frac{k_m^*(T_w, \lambda_m)}{k_m^*(T, \lambda_m)} \frac{k_m}{\lambda_m(k_m)} f_m(T, \phi, k_m) I_{bw} \exp(-\lambda_m s) dk_m \quad (23)$$

By comparison with the expression for I_{m1} in Eq. (14), it is clear that if

$$\mu_m = \frac{k_m^*(T_w, \lambda_m)}{k_m^*(T, \lambda_m)} \frac{k_m}{\lambda_m(k_m)} \quad (24)$$

then I_{m1} equals I_{m1}^* . Note that in the limit of $s=0$,

$$\sum_m \int_0^\infty \mu_m f_m dk_m = \sum_m \int_0^\infty \frac{k_m^*}{k} dk = 1 \quad (25)$$

i.e., the modified definition of μ_m satisfies Eq. (13) in an integral sense.

In Eq. (24), the overlap coefficient λ_m must be calculated in any case with or without wall emission and it is determined implicitly from Eq. (22). A convenient way of calculating the left- and right-hand side of Eq. (22) using a database of narrow-band k -distributions has been developed [11]. For a mixture of two gases, Eq. (22) reduces to the following equation to determine, for example, the λ_1-k_1 relation for gas 1 [11]:

$$\sum_{i=1}^{N_{nb}} \frac{I_{bi}}{I_b} \int_0^{g_{1,i}(k_1)} k_{1,i} dg_{1,i} = \sum_{i=1}^{N_{nb}} \frac{I_{bi}}{I_b} \int_{g_{1,i}=0}^1 k_{1,i} g_{2,i} (\lambda_1 - k_{1,i}) dg_{1,i} \quad (26)$$

where $k_{1,i}-g_{1,i}$ is the $k-g$ distribution for the i th narrow band, N_{nb} is the number of narrow bands comprising the entire spectrum, and the NB Planck function I_{bi} is defined as

$$I_{bi} = \int_{\Delta\eta_i} I_{b\eta} d\eta \quad (27)$$

A similar equation can be obtained for gas 2. In the narrow-band $k-g$ database published by Wang and Modest [16], the data are organized in such a way that the narrow-band $k-g$ pairs obtained from the database for a certain condition correspond to the quadrature points of a Gaussian quadrature scheme. Therefore, the integrals in Eq. (26) can be evaluated efficiently based on the narrow-band database.

For the ratio of k_m^* in Eq. (24), a formula that is similar to the evaluation of the right-hand side (RHS) of Eq. (26) can be derived to calculate k_m^* using the same narrow-band database. Alternatively, k_m^* can be determined by differentiating the RHS of Eq. (22), which must be calculated for the determination of λ_m . The alternative approach was found to be accurate and robust and was implemented as follows: The RHS is calculated from Eq. (26) for

a set of λ_m values using the narrow-band database; since it is a monotonically increasing function of λ_m , a monotonic cubic spline can be constructed readily; then the polynomial coefficients for the first-order term are the k_m^* for the corresponding λ_m values. Thus, with the above-noted considerations all terms in Eq. (24) can be evaluated efficiently from a narrow-band k - g database. Note that k_m^* needs to be evaluated twice, at both T_w and T .

In summary, the wall emission distribution scheme, Eq. (5), introduces the boundary emission distribution function μ_m in the MSFSK formulation. The coefficient μ_m can be evaluated by two approaches: from the direct definition, Eq. (13), and from the modified definition, Eq. (24). MSFSK calculations using the directly calculated μ_m may not recover the LBL result for a homogeneous medium bounded by a gray wall at a different temperature from that of the medium, due to the approximation made for λ_m . In addition, the direct approach involves line-by-line integration of the absorption coefficient and is, therefore, impractical for engineering applications. On the other hand, MSFSK calculations using the modified μ_m from Eq. (24) recover the LBL result for homogeneous media with arbitrary boundary wall temperatures, since it is formulated to incorporate the approximation made for λ_m . In addition, the modified approach can utilize a database of narrow-band k -distributions and is, therefore, efficient for practical problems. While the direct μ_m does not depend on gas temperature, the modified μ_m does since it incorporates the temperature-dependent overlap coefficient, in order to ensure that the radiative heat transfer in a homogenous medium is predicted correctly. If the gas is nonisothermal, then the modified μ_m is evaluated at the reference temperature.

Validation of Approach. In order to verify the accuracy of the two methods to calculate the boundary emission distribution function μ_m , the radiative heat flux emerging from a homogeneous layer (by volume 20% CO₂, 20% H₂O, and 60% N₂) bounded by a gray, diffuse emitting wall is calculated by both the MSFSK and the LBL method. LBL calculations provide the benchmark for the validation of the MSFSK method. In LBL calculations, the HITEMP [17] and CSDS [18] spectral databases are used for the absorption coefficients of H₂O and CO₂, respectively. In the MSFSK calculations, the k - g distributions and the nongray stretching functions a_m are constructed directly from the spectral absorption coefficients; the reference states are determined according to the formulas in Modest and Zhang [3]. For the purpose of validation, the distribution function μ_m , from both the direct formula, Eq. (13), and the modified formula, Eq. (24), are calculated directly from the absorption coefficient of the medium. The same is true for the evaluation of the overlap coefficient λ_m . The layer has a thickness of 50 cm and the wall temperature varies from 300 K to 2000 K. The calculated nondimensional exiting heat fluxes and the percentage errors of the MSFSK calculations compared to the LBL results are plotted in Fig. 1 for a medium temperature of 1000 K. The error is defined as

$$\text{Error} = \frac{\text{MSFSK} - \text{LBL}}{\text{LBL}} \times 100\% \quad (28)$$

It is shown that the modified- μ_m MSFSK calculations (green dash-dot lines) show small (less than 0.5%) errors, indicating that the modified μ_m are correctly formulated. The MSFSK calculations using the direct μ_m function show slightly larger errors. Within the wall temperature range considered, however, the error of using the directly calculated μ_m is still reasonably small.

Sample Calculations

To evaluate the distribution strategy of treating wall emission in the MSFSK method, and to illustrate the performance of the two approaches of computing the boundary emission distribution function μ_m , a few sample calculations were performed. In all cases, a mixture of CO₂-H₂O-N₂ confined between a hot gray wall and a

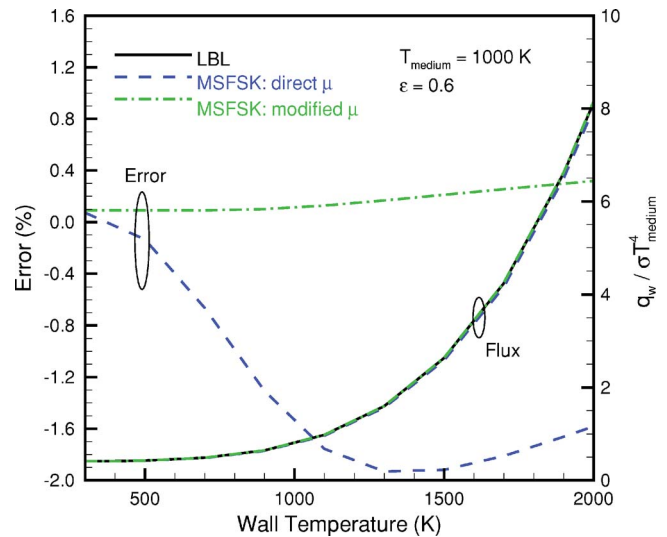


Fig. 1 Nondimensional heat flux leaving a homogeneous layer containing 20% CO₂ and 20% H₂O at 1000 K

cold black wall was considered. The mixture was at a total pressure of 1 bar and consists of two different homogeneous layers (denoted as left and right layer/column). Both layers had a fixed width of 50 cm. The hot gray wall was on the left and its temperature varies from 300 K to 2000 K while the right wall was kept cold and black. The left layer contained 20% CO₂ and 2% H₂O, and the right layer contained 2% CO₂ and 20% H₂O (i.e., the compositions are switched). The radiative heat flux leaving from the right layer and the radiative heat source within the medium were calculated using the LBL method, the MSFSK method with the direct and modified μ_m , and the (single scale) full-spectrum correlated- k (FSCK) method. The FSCK method was included in the calculations to demonstrate the improvement made by the MSFSK method.

In the MSFSK calculations, the direct μ_m were constructed from the medium absorption coefficient, while the modified μ_m were computed using the database of narrow-band k - g distributions by Wang and Modest [16], as outlined in the previous section. When the direct μ_m were used in the calculation, all other parameters, such as the k - g distribution, the stretching function a_m , and the overlap coefficient λ_m , were also constructed directly from the medium absorption coefficient. When the modified μ_m were used, they and all the other parameters were computed using the W&M narrow-band database [16]. In both FSCK and MSFSK calculations, the spectral integrations over g -space were performed using the trapezoidal rule together with all available data points in order to limit the error caused by numerical integration. Here 2000 data points were used in the FSCK and direct- μ_m MSFSK calculations, while only 128 points were available for the modified- μ_m MSFSK calculations, since the modified μ_m were constructed from the narrow-band database that contains at most 128 quadrature points for each of the narrow bands [16]. For practical applications of the MSFSK methods, an efficient quadrature scheme is desired, and therefore, a Gaussian quadrature scheme with 10 quadrature points was also employed for the modified- μ_m MSFSK calculations using the narrow-band database. The computational cost of FSCK calculations include CPU time for both RTE solution and assembly of k - g distributions from the narrow-band database. The MSFSK CPU time for RTE solutions will be M -fold (number of scales) larger than the FSCK CPU time, but remains only a tiny fraction of the LBL cost. Besides the assembly of k - g distributions, the MSFSK method also needs to compute the medium and wall emission overlap coefficients. It was found in the following sample calculations that the

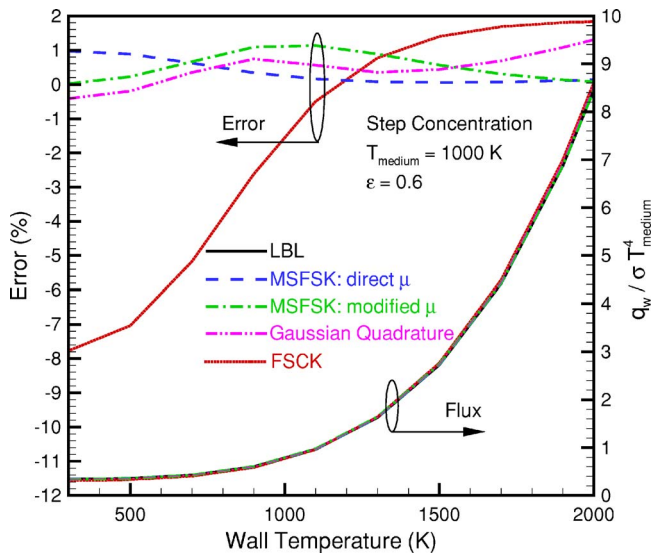


Fig. 2 Nondimensional heat flux leaving an inhomogeneous layer at 1000 K with step changes in mole fraction: 20% CO₂ and 2% H₂O in the left layer, with the composition switched in the right layer

computation of the medium and wall emission overlap coefficients each needs about the same CPU time as the assembly of k - g distributions, which is also M -fold larger than that required by FSCK.

Figure 2 shows the calculated nondimensional radiative heat fluxes for the case of severe step changes in gas concentration. The temperature of both layers was at a uniform 1000 K. Also shown in the figure are the percentage errors of the MSFSK and FSCK calculations compared to LBL results. In the MSFSK calculations, both the direct- and modified- μ approaches give small errors of less than 2%, and the direct- μ approach performs slightly better than the modified- μ approach for higher wall temperatures. In comparison, the FSCK method incurs much larger errors for low wall temperature, although the error decreases as wall emission becomes dominant. The better performance of the MSFSK method over the FSCK method shows that the multiscale scheme resolves the inhomogeneous problem due to partial pressure variations and the scheme is robust even under conditions of severe step changes. Figure 2 also demonstrates that the distribution scheme for wall emission and the formulation for the wall emission distribution function are successful.

The Gaussian quadrature evaluation with ten quadrature points, as also shown in Fig. 2, has the same order of accuracy as the direct integration. The choice of quadrature points, however, required some attention. In general, in a FSCK calculation the quadrature points are chosen such that more points are distributed toward larger g -values (corresponding to large k -values), since the larger k -values usually determine radiative heat transfer rates if the optical thickness of the medium is small to moderate. In the cases when wall emission becomes dominant, the part of the spectrum corresponding to smaller k -values is nearly transparent to wall emission. This requires the quadrature points to be distributed toward the smaller g -values as well. In the sample calculation, a Gauss-Chebyshev quadrature scheme was used that places more points symmetrically toward both ends of the g -range, 0 and 1. This quadrature scheme gives errors of less than 2% compared to the LBL results for a large range of wall temperatures (300 K to 2000 K).

Figure 3 shows the distribution of radiation heat loss for the same inhomogeneous medium as used in the previous calculations. Two different boundary conditions, cold black and hot gray at 2000 K, for the left wall bounding the medium were consid-

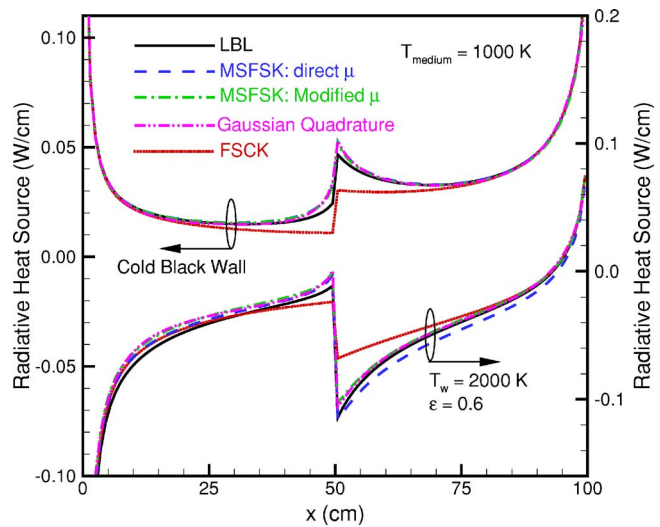


Fig. 3 Radiative heat source distribution for an inhomogeneous layer at 1000 K with step changes in mole fraction: 20% CO₂ and 2% H₂O in the left layer, with the composition switched in the right layer

ered. The distributions calculated again by LBL, MSFSK, and FSCK methods are compared in Fig. 3. Because of the step change in medium concentration, there is a discontinuity in the middle of the medium since H₂O is a stronger emitter and absorber than CO₂: without wall emission (upper jump) H₂O emits more energy than CO₂; with wall emission, H₂O absorbs more wall-emitted energy than CO₂. The FSCK method responds poorly to the step change in concentration and fails to capture the trend predicted by the LBL approach. The MSFSK methods, on the other hand, perform well in this severe case and follow closely the discontinuity caused by the step change in medium concentration. Note that, when radiative heat loss is calculated using Gaussian quadrature, the quadrature scheme need not put emphasis on the lower end of the g -values, since those spectral regions have small k -values and, therefore, negligible emission and absorption inside the medium. However, when radiation heat flux and heat source are calculated all at once, the quadrature scheme with emphasis on both ends of the g -values would be preferred.

Figure 4 shows the results for an even more severe case, in which a step change in temperature was added to the mixture's inhomogeneity together with step changes in gas concentration. The current MSFSK formulation does not deal with temperature inhomogeneities, which will be addressed in a follow-up paper. The error of the MSFSK method for media with temperature inhomogeneities has been discussed in the previous MSFSK development [11]. Here the focus is the treatment of boundary wall emission within the MSFSK method. It is seen from the figure that, even in the presence of a temperature inhomogeneity, the MSFSK method performs about five times better than the FSCK method, although, as expected, the advantage of the MSFSK method diminishes again as the wall temperature becomes large and wall emission dominates over medium emission. In the MSFSK calculations, the modified- μ approach performs equally well as the direct- μ approach, but it holds the advantage of efficiency derived from using a narrow-band k - g distribution database.

Summary and Conclusions

In this paper a distribution scheme for the treatment of boundary wall emission within the MSFSK method has been proposed. This scheme is consistent with the overlap concept of the MSFSK method and requires no changes in the original MSFSK formulation. A boundary emission distribution function has been introduced and two approaches to evaluate the function have been

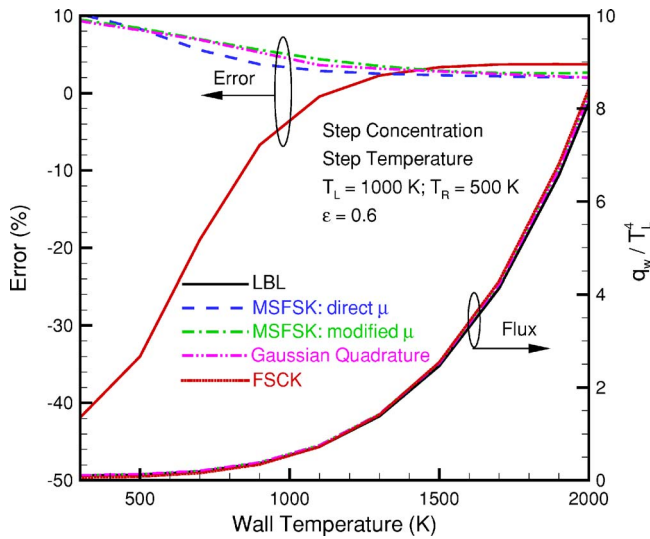


Fig. 4 Nondimensional heat flux leaving an inhomogeneous layer with step change in mole fraction and temperature: 20% CO₂ and 2% H₂O at 1000 K in the left layer and 2% CO₂ and 20% H₂O at 500 K in the right layer

derived: a direct approach and a modified approach. The wall emission distribution scheme and the two approaches were evaluated by performing sample calculations for radiative transfer in strongly inhomogeneous media. It was found that the distribution scheme successfully handled boundary wall emission of arbitrary temperature. The direct approach for the calculation of the boundary distribution function is somewhat cumbersome and does not recover LBL results for homogeneous media. The modified approach, on the other hand, is readily evaluated at no additional computational cost from the database of narrow-band k - g distributions used in the MSFSK scheme and does recover LBL results for homogeneous media. For inhomogeneous media, the modified approach performs equally well as the direct approach.

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Nomenclature

- a = stretching factor for FSK method
- f = k -distribution function (cm)
- g = cumulative k -distribution
- I = radiative intensity (W/m²sr)
- k = absorption coefficient variable (cm⁻¹)
- k^* = overlap parameter defined in Eq. (19)
- L = geometric length (cm)
- M = total number of scales
- \hat{n} = surface normal
- P = pressure, bar
- q = radiative heat flux (W/m²)
- s = distance along path (cm)
- \hat{s} = unit direction vector
- T = temperature (K)
- x, x = mole fraction (vector)

Greek Symbols

- η = wave number (cm⁻¹)
- ϕ = composition variable vector

- δ = Dirac's delta function
- λ = overlap coefficient defined in Eq. (11), cm⁻¹
- μ = boundary emission distribution function defined in Eq. (13)
- κ = absorption coefficient (cm⁻¹)
- ϵ = wall emittance
- Ω = solid angle (sr)
- σ = Stefan-Boltzmann constant

Subscripts

- 0 = reference condition
- b = blackbody emission
- g = spectral in g -space
- i = i th narrow band
- L = left layer
- m = m th scale
- R = right layer
- w = wall
- η = spectral in wave-number space

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