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MULTI-SCALE FULL-SPECTRUM k-DISTRIBUTION METHOD FOR RADIATIVE TRANSFER IN INHOMOGENEOUS GAS MIXTURES WITH WALL EMISSION

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ABSTRACT

The multi-scale full-spectrum k-distribution (MSFSK) method has become a promising method for radiative heat transfer in inhomogeneous media. In this paper an original distribution scheme is proposed to extend the MSFSK's ability in dealing with boundary wall emission. This scheme pursues the overlap concept of the MSFSK method and requires no changes in the original MSFSK formulation. A boundary emission overlap coefficient is introduced and two approaches of evaluating the coefficient are outlined. The distribution scheme 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.

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

Nomenclature

a	stretching factor for FSK method
f	k-distribution function, cm
g	cumulative k-distribution
I	radiative intensity, W/m^{2}sr
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/m^2
s	distance along path, cm
$\hat{s}$	unit direction vector
T	temperature, K
$x, \underline{x}$	mole fraction (vector)

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}
μ	boundary emission overlap coefficient defined in Eq. (13)
κ	absorption coefficient, cm^{-1}
ϵ	wall emissivity
Ω	solid angle, sr
σ	Stefan–Boltzmann constant

Subscripts

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

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Introduction

Because of the strongly irregular spectral variations of gas absorption coefficients, the line-by-line (LBL) approach generally has to be 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 remains, 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 Riviere et al. [6–8] and by Modest and Zhang [3]. They are the focus of further FSK developments.

The multi-group FSK (MGFSK) [9] and multi-scale 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 multi-scale 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 (SLW) methods [**?**], is limited to media surrounded by cold, non-emitting 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 the original MSFSK formulation unchanged. The mathematical development for the boundary scheme is described, followed by validation of the approach. Sample calculations are performed for a mixture with extremely 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 radiative transfer equation (RTE) is then written as [12]

$$\frac{\mathrm{d}I_\eta}{\mathrm{d}s} = \kappa_\eta(\underline{\phi})(I_{b\eta} - I_\eta), \tag{1}$$

subject to the boundary condition

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

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 $\underline{\phi}$ contains 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 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 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.,

$$\kappa_\eta = \sum_{m=1}^{M} \kappa_{m\eta}, \quad I_\eta = \sum_{m=1}^{M} I_{m\eta}, \tag{3}$$

then the RTE (1) is transformed into M component RTE's, 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

$$\frac{\mathrm{d}I_{m\eta}}{\mathrm{d}s} = \kappa_{m\eta}(\underline{\phi})I_{b\eta} - \kappa_{\eta}(\underline{\phi})I_{m\eta}, \quad \text{for } m = 1,\ldots,M. \tag{4}$$

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 equation (4), if there is no wall emission, the spectral locations where κ_η contributes to the absorption of $I_{m\eta}$ are only those wavenumbers for which $\kappa_{m\eta}$ is nonzero. The overlap region is only a subset of those wavenumbers 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 region for each scale is relatively small compared to the total emission/absorption spectrum of each scale. If there is wall emission, however, the underlying assumptions of the MSFSK scheme are no longer valid and large errors may appear.

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,

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

where $\underline{\phi}_0$ denotes the reference state of the mixture. Note that the sum of equation (5) over all the scales reduces to equation (2). With such distribution, wall emission exists within each scale only at the spectral locations where the 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 [13] to the RTE of each scale: first equation (4) is multiplied by Dirac's delta function $\delta(k_m - \kappa_{m\eta}(\underline{\phi}_0))$, followed by division with the k-distribution of the m-th scale, or

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

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

$$\frac{\mathrm{d}I_{mg}}{\mathrm{d}s} = k_m(T_0,\underline{\phi},g_m)a_m I_b - \lambda_m I_{mg}, \quad \text{for } m = 1,\ldots,M, \tag{7}$$

where

$$I_{mg} = \int_0^\infty I_{m\eta}\delta\left(k_m - \kappa_{m\eta}(\underline{\phi}_0)\right)\mathrm{d}\eta \Big/ f_m(T_0,\underline{\phi}_0,k_m), \tag{8}$$

$$g_m = \int_0^{k_m} f_m(T_0,\underline{\phi}_0,k)\mathrm{d}k \tag{9}$$

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

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

Here the correlated-k (FSCK) approach has been taken [13]. 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 [equation (5)], one obtains the reordered condition corresponding to equation (7):

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

where

$$\mu_m = \frac{1}{I_{bw}} \int_0^\infty \frac{\kappa_{m\eta}(\underline{\phi}_0)}{\kappa_\eta(\underline{\phi}_0)} I_{b\eta w} \delta\left(k_m - \kappa_{m\eta}(\underline{\phi}_0)\right) \mathrm{d}\eta \Big/ f_m(T_0, \underline{\phi}_0, k_m). \tag{13}$$

Here μ_m is the boundary emission overlap coefficient and can be evaluated from equation (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 equation (7) for a homogeneous mixture bounded by a black wall may be written as

$$\begin{aligned} I_m &= \int_0^1 I_{mg} \mathrm{d}g \\ &= \int_0^\infty \mu_m I_{bw} \exp(-\lambda_m s) f_m(T, \underline{\phi}, k_m) \mathrm{d}k_m + \\ &\quad \int_0^\infty \frac{k_m}{\lambda_m} I_b \left[1 - \exp(-\lambda_m s)\right] f_m(T, \underline{\phi}, k_m) \mathrm{d}k_m \\ &= I_{m1} + I_{m2}, \end{aligned} \tag{14}$$

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

$$\frac{\mathrm{d}I^*_{mg}}{\mathrm{d}s} = \frac{k^*_m(T) I_b}{f(T, \underline{\phi}, k)} - k I^*_{mg}, \quad \text{for } m = 1, \ldots, M, \tag{15}$$

and the corresponding boundary condition,

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

where

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

$$I^*_{mg} = \int_0^\infty I_{m\eta} \delta\left(k - \kappa_\eta(\underline{\phi})\right) \mathrm{d}\eta \Big/ f(T, \underline{\phi}, k), \tag{18}$$

$$k^*_m(T) = \frac{1}{I_b(T)} \int_0^\infty I_{b\eta}(T) \kappa_{m\eta} \delta\left(k - \kappa_\eta(\underline{\phi})\right) \mathrm{d}\eta. \tag{19}$$

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

$$\begin{aligned} I^*_m &= \int_0^1 I^*_{mg} \mathrm{d}g \\ &= \int_0^\infty \frac{k^*_m(T_w)}{k} I_{bw} \exp(-ks) \mathrm{d}k + \int_0^\infty \frac{k^*_m}{k} I_b \left[1 - \exp(-ks)\right] \mathrm{d}k \\ &= I^*_{m1} + I^*_{m2}, \end{aligned} \tag{20}$$

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]

$$\lambda_m = k \quad \text{and} \quad k_m f_m(T, \underline{\phi}, k_m) \mathrm{d}k_m = k^*_m(k) \mathrm{d}k. \tag{21}$$

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

$$\int_0^{k_m} k'_m f_m(T, \underline{\phi}, k'_m) \mathrm{d}k'_m = \int_0^{k'=\lambda_m} k^*_m(k') \mathrm{d}k'. \tag{22}$$

In the presence of wall emission I_{m1} may, in general, not be equal to I^*_{m1} if λ_m is determined from equation (22), since the equation is derived from considering medium emission only. In addition, the evaluation of μ_m from equation (13) appears to be inconvenient. We can, however, modify the definition for μ_m, equation (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 very easily, as shown below.

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

$$\begin{aligned} I^*_{m1} &= \int_0^\infty \frac{k^*_m(T_w)}{k^*_m(T)} \frac{k^*_m(T)}{k} I_{bw} \exp(-ks) \mathrm{d}k \\ &= \int_0^\infty \frac{k^*_m(T_w)}{k^*_m(T)} \frac{k_m}{\lambda_m} f_m(T, \underline{\phi}, k_m) I_{bw} \exp(-\lambda_m s) \mathrm{d}k_m. \end{aligned} \tag{23}$$

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

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

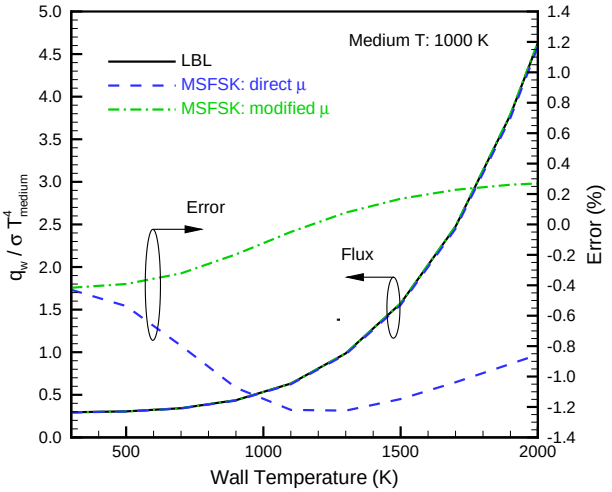

Figure 1. **Nondimensional heat flux leaving a homogeneous layer of 20% CO_2 and 20% H_2O at 1000 K.**

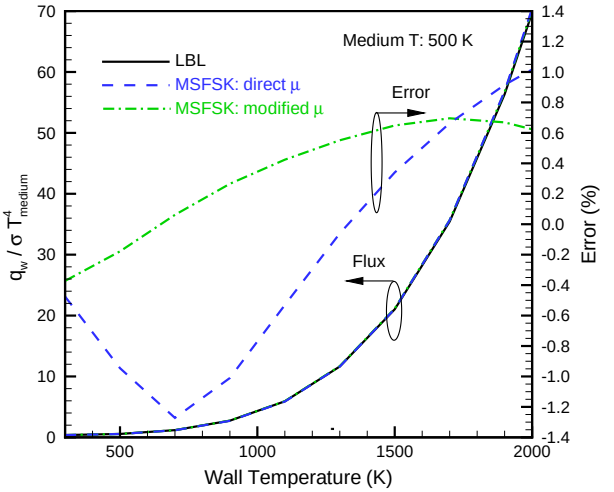

Figure 2. **Nondimensional heat flux leaving a homogeneous layer of 20% CO_2 and 20% H_2O at 500 K.**

then I_{m1} equals I^*_{m1}.

The k^*_m in equation (24) are also needed for the evaluation of λ_m and a convenient way of calculating k^*_m using a database of narrow-band k-distributions has already been developed [11]. Thus equation (24) is readily evaluated.

Validation of Approach

The boundary emission overlap coefficient μ_m can be evaluated directly from its definition, equation (13), but the MSFSK calculation using the directly calculated μ_m may not recover the LBL result for a homogeneous medium bounded by a black wall at a different temperature from that of the medium, due to the approximation made for λ_m. Equation (24) provides a modification for μ_m, incorporating the original approximation of λ_m for homogeneous media without wall emission, such that the MSFSK method using the original λ_m and modified-μ_m will predict the same result as LBL calculations for homogeneous media with arbitrary boundary wall temperatures.

In order to verify the accuracy of the two methods to calculate the boundary emission overlap coefficient μ_m, the radiative heat flux emerging from a homogeneous layer (by volume 20% CO_2, 20% H_2O, and 60% N_2) bounded by a black emitting wall is calculated by both the MSFSK and and the LBL method. LBL calculations provide the benchmark for validating the MSFSK method. In LBL calculations, the HITEMP [14] and CDSD [15] spectral databases are used for the absorption coefficients of H_2O and CO_2, respectively. In the MSFSK calculations, the k–g distributions are constructed directly from the spectral databases; the reference states and the scaling functions are determined according to the formulas in Modest and Zhang [3] The coefficient μ_m are computed using both the direct formula, equation (13), and the modified formula, equation (24). 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 errors of the MSFSK calculations compared to the LBL results are plotted in Figs. 1 and 2 for two medium temperatures, 1000 K and 500 K, respectively. In both cases, the modified μ 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 coefficients show slightly larger errors. Within the wall temperature range considered, however, the error of using the directly calculated μ_m is still reasonably small. In fact, using the direct-calculated μ_m shows slightly better agreement with LBL results for the inhomogeneous cases as will be shown in the following section.

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 overlap coefficient μ_m, a few sample calculations are performed. In all cases, we will consider a mixture of CO_2–H_2O–N_2 confined between a hot and a cold black wall. The mixture is at a total pressure of 1 bar and consists of two different homogeneous layers (denoted as left and right layer/column). Both layers have a fixed width of 50 cm. The hot black wall is on the left and its temperature varies from 300 K to 2000 K while the right wall is kept cold. The left layer contains 20% CO_2 and 2% H_2O, and the right layer contains 2% CO_2 and 20% H_2O (i.e., the composition

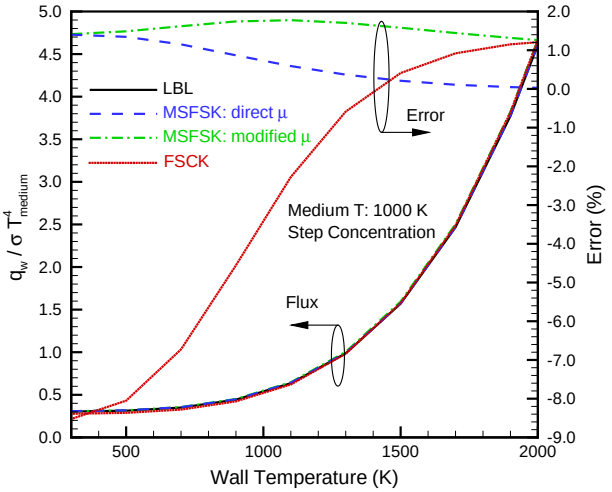

Figure 3. **Nondimensional heat flux leaving an inhomogeneous layer at 1000 K with step changes in mole fraction: 20% CO_2 and 2% H_2O in the left layer and the composition switched in the right layer.**

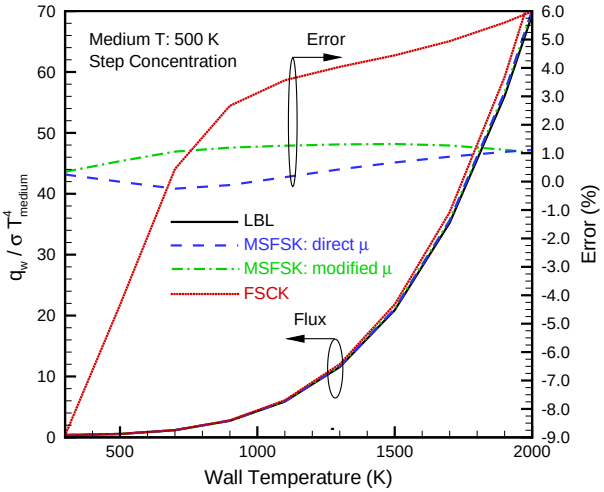

Figure 4. **Nondimensional heat flux leaving an inhomogeneous layer at 500 K with step changes in mole fraction: 20% CO_2 and 2% H_2O in the left layer and the composition switched in the right layer.**

is switched). The radiative heat flux leaving from the right layer is 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 is included in the calculations to demonstrate the improvement made by the MSFSK method.

Figure 3 shows the calculated nondimensional radiative heat fluxes for the case of severe step changes in gas concentration. The temperature of both layers is 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 consistently better than the modified-μ approach for different hot wall temperatures. In comparison, the FSCK method predicts much larger errors for low wall temperature, although the error decreases as wall emission becomes dominant. However, if the uniform medium temperature is reduced to 500 K, the FSCK calculations deviate strongly from LBL results for most of the wall temperatures, as shown in Fig. 4. The MSFSK calculations, on the other hand, remain close to LBL results with errors less than 1.5%. Again, for the lower medium temperature, the direct-μ approach slightly outperforms the modified-μ approach.

Figure 5 shows the results for an even more severe case, in which a step change in temperature is added to the mixture's inhomogeneity 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 with the presence of temperature inhomogeneity, the MSFSK method performs about 5 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. Once again in the MSFSK calculations, the direct-μ approach provides a slightly better result than the modified-μ approach.

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 require no changes in the original MSFSK formulation. A boundary emission overlap coefficient has been introduced and two approaches to evaluate the coefficient have been outlined. The distribution scheme and the two approaches are 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 of calculating the boundary overlap coefficient is somewhat cumbersome and does not recover LBL results for homogenous media. The modified approach, on the other hand, is readily evaluated at no

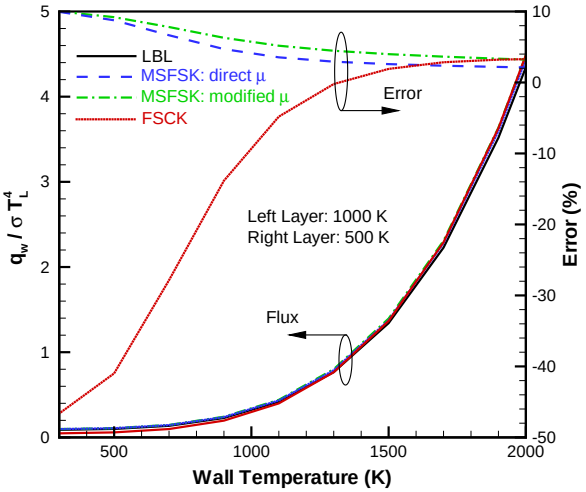

Figure 5. **Nondimensional heat flux leaving an inhomogeneous layer with step change in mole fraction and temperature: 20% CO_2 and 2% H_2O at 1000K in the left layer and 2% CO_2 and 20% H_2O at 500K in the right layer.**

additional computational cost and does recover LBL results for homogeneous media, although for inhomogeneous media, it is slightly less accurate than the direct approach.

Acknowledgments

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