JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 27, No. 3, July–September 2013

Technical Notes

k-Distribution Methods for Radiation Calculations in High-Pressure Combustion

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DOI: 10.2514/1.T3957

Nomenclature

a = nongray stretching factor for fill-spectrum *k*-distribution method
I = radiative intensity, $\mathrm{W/m^2\ sr}$
I_b = blackbody intensity/Planck function, $\mathrm{W/m^2\ sr}$
k = reordered absorption coefficients in *k* distribution, $\mathrm{cm^{-1}}$
L = length of one-dimensional medium, cm
M = total number of groups of *n*th gas component
N = total number of species/scales
P = total pressure, bar
PL = pressure path length, $P \times L$, bar-cm
q = heat flux, $\mathrm{W/m^2}$
$\hat{\mathbf{s}}$ = unit direction vector
T = temperature, K
$\underline{x}$ = gas species mole fraction
η = wave number, $\mathrm{cm^{-1}}$
κ = absorption coefficient, $\mathrm{cm^{-1}}$
λ = overlap parameter, $\mathrm{cm^{-1}}$
σ_s = scattering coefficient, $\mathrm{cm^{-1}}$
τ = narrow-band transmissivity
Φ = scattering phase function
$\boldsymbol{\phi}$ = composition variable vector
Ω = solid angle, sr

Subscripts

b = blackbody function
g = cumulative *k* distribution
m = *m*th group of *n*th gas/scale
n = *n*th gas/scale

I. Introduction

NONGRAY radiation calculations in participating media can be most accurately performed using the line-by-line (LBL) approach. The LBL approach requires in excess of one million spectral solutions of the radiative transfer equation (RTE) during radiation calculations in the combustion system [1–5], making such radiation calculations prohibitive. For accurate and computationally efficient solutions of the RTE, several models have been proposed, applying the concept of reordering the absorption coefficient across the entire spectrum. These include the spectral-line-based weighted-sum-of-gray-gases (SLW) model [6,7], the absorption distribution function (ADF) method [8,9], and the full-spectrum *k*-distribution (FSK) method [10,11]. The SLW and ADF methods are approximate schemes, in which the absorption coefficient is reduced to a few discrete values (chosen by the user), and integration over the spectrum is achieved by adding contributions of the "gray gases" (effectively trapezoidal rule quadrature, which requires a large number of points for good accuracy). The FSK method, on the other hand, is an exact method for a correlated absorption coefficient using a continuous *k* distribution over the entire spectrum. Spectral integration can be performed using high-accuracy Gaussian quadrature, which generally yields excellent accuracy for less than half the number of points required by the trapezoidal rule of integration. Several advancements for the *k*-distribution method have been proposed to address the shortcomings of the basic FSK scheme in strongly inhomogeneous media based on the multiscale (MS) [2] and the multigroup (MG) approaches [12], which may be summarized as 1) the full-spectrum-based hybrid multiscale multigroup FSK (MSMGFSK) method [13] (accommodates temperature and concentration inhomogeneities but only for gas mixtures), 2) the narrowband-based MSFSK method [14] for nongray multiphase mixtures with/without gray wall emission (accommodates concentration inhomogeneity), and 3) the narrowband-based hybrid MSMGFSK method [15] for nongray multiphase mixtures with/without wall emission (accommodates both temperature and concentration inhomogeneities). Recently, a portable spectral module has been developed by Pal and Modest [16] incorporating the LBL method and all of the *k*-distribution methods with corresponding *k*-distribution databases to facilitate spectral radiation calculations.

Radiation calculations with high-accuracy spectral modeling of gas properties in elevated pressure systems are scarce in literature. Denison and Webb showed good agreement in the emissivity calculation of a gas mixture at higher than atmospheric pressure compared to experimental measurements using the absorption-line blackbody distribution function in the SLW method [17]. However, almost all high-fidelity *k*-distribution-based spectral radiation models have been developed for atmospheric pressure combustion [18]. In current FSK models, *k-g* distributions for a mixture are constructed on the fly using a high-accuracy database of single-species *k* distributions together with a narrowband (NB) mixing model [19]. The NB mixing model [19] assumes that, at the NB level, the absorption coefficients of gases are uncorrelated (due to their small overlap), and hence the transmissivities of gases are multiplicative. The same assumption is also invoked during overlap parameter calculations in multiscale fill-spectrum *k*-distribution (MSFSK) and MSMGFSK models.

At elevated pressure, where radiation becomes more dominant, stronger line overlap among various gaseous species is likely. Under such circumstances, the multiplicative rule of gas transmissivities may incur inaccuracies; hence, the accuracy of the mixing model needs to be validated at higher pressure. The objective of this Note is to investigate the performance of *k*-distribution methods in conjunction with the mixing model for high-pressure conditions. The accuracy of mixing models in various FSK methods was tested for one-dimensional (1-D) homogeneous and inhomogeneous media and a two-dimensional (2-D) axisymmetric medium involving combustion of methane. All *k*-distribution methods studied in this Note assume correlated absorption coefficients; thus, the "correlated" term

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Presented as Paper 2012-529 at the 50th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition, Nashville, TN, 9–12 January 2012; received 22 May 2012; revision received 19 March 2013; accepted for publication 21 March 2013; published online 17 June 2013. Copyright © 2013 by the American Institute of Aeronautics and Astronautics, Inc. All rights reserved. Copies of this paper may be made for personal or internal use, on condition that the copier pay the $10.00 per-copy fee to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923; include the code 1533-6808/13 and $10.00 in correspondence with the CCC.

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is not repeatedly used: for example, FSK represents full-spectrum correlated *k*-distribution method.

II. Radiation Models

The *k*-distribution method reorders the rapidly oscillating absorption coefficient across the spectrum into a well-behaved smooth monotonically increasing function vs a cumulative distribution function g, which acts as a nondimensional wave number. The tedious integration over wave number space can then be replaced by integration over g space using a small number of quadrature points. The RTE for an emitting–absorbing–scattering medium on a spectral basis can be written as [20]

$$\frac{\mathrm{d}I_\eta}{\mathrm{d}s} = \kappa_\eta(\underline{\boldsymbol{\phi}})I_{b\eta} - (\kappa_\eta(\underline{\boldsymbol{\phi}}) + \sigma_{s\eta}(\underline{\boldsymbol{\phi}}))I_\eta + \frac{\sigma_{s\eta}(\underline{\boldsymbol{\phi}})}{4\pi}\int_{4\pi} I_\eta(\hat{\mathbf{s}}')\Phi_\eta(\underline{\boldsymbol{\phi}})(\hat{\mathbf{s}},\hat{\mathbf{s}}')\,\mathrm{d}\Omega' \tag{1}$$

where κ_η and $\sigma_{s\eta}$ are the spectral absorption and scattering coefficients, respectively. The vector $\underline{\boldsymbol{\phi}}$ contains state variables that affect κ_η and $\sigma_{s\eta}$, which include temperature T, total pressure P, and gas mole fractions $\underline{x}$: $\underline{\boldsymbol{\phi}} = (T, P, \underline{x})$. A unit direction vector is $\hat{\mathbf{s}}$, and Φ_η is the spectral scattering phase function. In the most advanced FSK method, i.e., the MSMGFSK method [15], the mixture's spectral absorption coefficient κ_η is first separated into contributions from N species, and then the spectral locations of the nth gas absorption coefficient are sorted into M exclusive spectral groups: that is,

$$\kappa_\eta = \sum_{n=1}^{N}\sum_{m=1}^{M_n}\kappa_{nm\eta}, \qquad I_\eta = \sum_{n=1}^{N}\sum_{m=1}^{M_n} I_{nm\eta} \tag{2}$$

The radiative intensity I_η is also broken up accordingly. The RTE [Eq. (1)] is then transformed into

$$\sum_{n=1}^{N} M_n$$

component RTEs: one for each group of each species scale (assuming gray scattering):

$$\frac{\mathrm{d}I_{nm\eta}}{\mathrm{d}s} = \kappa_{nm\eta}I_{b\eta} - (\kappa_\eta + \sigma_s)I_{nm\eta} + \frac{\sigma_s}{4\pi}\int_{4\pi} I_{nm\eta}(\hat{\mathbf{s}}')\Phi(\hat{\mathbf{s}},\hat{\mathbf{s}}')\,\mathrm{d}\Omega', \quad \text{for } n = 1,\ldots,N; \quad m = 1,\ldots,M_n \tag{3}$$

Note that the intensity $I_{nm\eta}$ is due to emission by the mth group of the nth scale (the nmth group) but subject to absorption by all groups of the other scales and its own group. The FSK reordering is done by multiplying Eq. (3) by a Dirac-delta function, followed by integration over the entire spectrum [15] as

$$\frac{\mathrm{d}I_{nmg}}{\mathrm{d}s} = k_{nmg}a_{nmg}I_b - (\lambda_{nmg} + \sigma_s)I_{nmg} + \frac{\sigma_s}{4\pi}\int_{4\pi} I_{nmg}(\hat{\mathbf{s}}')\Phi(\hat{\mathbf{s}},\hat{\mathbf{s}}')\,\mathrm{d}\Omega', \quad \text{for } n = 1,\ldots,N; \quad m = 1,\ldots,M_n \tag{4}$$

where a_{nmg} is a nongray stretching factor, and λ_{nmg} is the overlap parameter for the mth group of the nth scale (details can be obtained from Pal and Modest [15]). From the MSMGFSK method, a single-group MSFSK method (with N scales) can also be obtained by letting $M_n = 1$, and the basic single-group–single-scale FSK method is retrieved by setting $M_n = N = 1$ (and $\lambda_g = k_g$). Details of the NB-based k-g-distribution mixing model can be obtained from Modest and Riazzi [19].

III. Results

The mixing model and the FSK methods were tested for various 1-D and 2-D problems for pressures up to 30 bar. Figure 1 shows the absolute errors $(\tau_{\eta,\mathrm{LBL\,direct}} - \tau_{\eta,\mathrm{LBL\,mixing}})$ in NB transmissivity calculations using the current mixing rule for a medium of path length of 2 m at 1500 K containing important combustion gases such as CO_2 and H_2O (1% CO_2 and 2% H_2O). For *k*-distribution-based calculations, narrowband-based data were obtained from databases compiled by Wang and Modest [21], while LBL data were obtained from spectroscopic databases, such as CDSD-1000 for CO_2 [22], HITEMP (high temperature) for H_2O [23], and HITRAN (high-resolution transmission) for all other gases. [24] Since CO_2 and H_2O overlap primarily at the trailing edge of the 2.7 μm band, the errors in transmissivity calculations are highest at this spectral location (as shown); everywhere else, errors are negligibly small. NB transmissivities calculated using the mixing rule and single-species *k*-distribution databases $(\tau_{\eta,\mathrm{DB\,mixing}})$ are essentially identical to LBL-mixing values, i.e., $\tau_{\eta,\mathrm{LBL\,mixing}}$ (not shown). Although the mixing rule incurs some errors near 3400 cm^{-1}, due to its extremely localized nature, this has no significant effect on heat transfer calculations.

A 1-D homogeneous isothermal layer of gas mixture (1% CO_2 and 2% H_2O by mole) bounded by cold black walls at various pressures was considered, keeping the pressure path length constant at 200 bar · cm. For such a homogeneous medium, the *k*-distribution method is exact, and hence is expected to yield results within the accuracy of the integration scheme (typically 0.5%). Any error in addition to the quadrature error will be due to the mixing rule to construct the mixture *k*-*g*-distribution from individual *k*-*g*-distributions. The nondimensional heat fluxes exiting the medium were calculated using the line-by-line, FSK, and more advanced models, such as the multiscale FSK in conjunction with the analytical solution of RTE in 1-D medium (see details for [20]). Relative errors are determined by comparison with LBL method as

$$\mathrm{error}(\%) = \frac{q_{\mathrm{LBL}} - q_{\mathrm{FSK/MSFSK}}}{q_{\mathrm{LBL,max}}} \times 100 \tag{5}$$

The results are tabulated in Table 1. It is seen that errors in heat flux calculations using FSK and MSFSK methods are always negligibly small compared to the LBL calculations and limited to 1%. At atmospheric pressure, the MSFSK method consistently yields higher accuracy for homogeneous media compared to higher pressures. The explanation for such observation is that, as the pressure increases, the width of the absorption lines broaden, increasing the overlap among species. One of the basic assumptions of the MSFSK method is that overlap among species is small, which is less accurate at higher pressure. Thus, the MSFSK method incurs more inaccuracy (although very small in magnitude) in heat transfer for homogeneous media at higher pressure compared to its atmospheric counterpart.

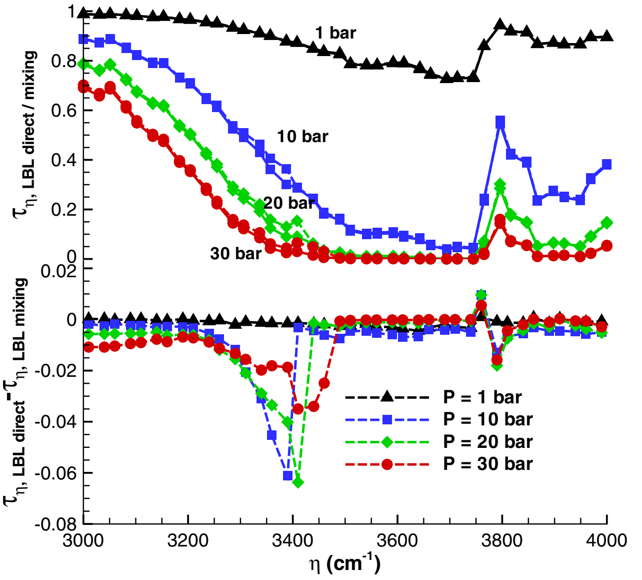

Fig. 1 Comparison of NB transmissivities calculated directly and using mixing rule (solid line: direct, dashed line: mixing rule).

Table 1 Nondimensional heat flux exiting homogeneous isothermal medium at various pressures

T, K	$P \times L$, bar · cm	LBL	FSK	MSFSK	Error FSK, %	Error MSFSK, %
500	1 bar × 200 cm	0.2134	0.2142	0.2133	0.37	−0.05
	10 bar × 20 cm	0.3325	0.3348	0.3354	0.69	0.87
	20 bar × 10 cm	0.3631	0.3652	0.3662	0.58	0.85
	30 bar × 6.667 cm	0.3916	0.3936	0.3945	0.51	0.76
1000	1 bar × 200 cm	0.1748	0.1748	0.1749	0.01	0.07
	10 bar × 20 cm	0.2338	0.2351	0.2361	0.56	0.98
	20 bar × 10 cm	0.2474	0.2483	0.2499	0.36	1.01
	30 bar × 6.667 cm	0.2551	0.2556	0.2577	0.20	1.00
1500	1 bar × 200 cm	0.1224	0.1227	0.1225	0.27	0.08
	10 bar × 20 cm	0.1486	0.1485	0.1491	−0.07	0.34
	20 bar × 10 cm	0.1538	0.1537	0.1551	−0.70	0.85
	30 bar × 6.667 cm	0.1602	0.1589	0.1618	−0.81	0.98

The accuracy of k-distribution methods was investigated for an inhomogeneous medium at high pressure. A 1-D medium containing a CO_2-H_2O gas mixture, confined between cold black walls, was considered. The mixture consisted of two different homogeneous layers (denoted as left/hot and right/cold layers) adjacent to each other with step changes in the temperatures and concentrations of the species. Two different total pressures of 1 and 30 bar were considered. The pressure path length of the left/hot layer was kept constant at 60 bar · cm, while the pressure path length was varied for the right/cold layer. Such problems with step changes in species concentration and/or temperature provide an acid test for these methods because of their extreme inhomogeneity gradients. Figure 2 shows the results for the case where the left layer contained 10% CO_2, 20% H_2O at 1500 K, whereas the right layer contained 20% CO_2, 10% H_2O at 300 K. It is seen that the MSFSK method calculations are more accurate (approximately by a factor of 4) than the single-scale FSK method results for both pressures. The accuracy of both methods increases with increase in pressure, which can be due to the larger optical thickness and the increase in line broadening resulting in a smoother absorption coefficient profile.

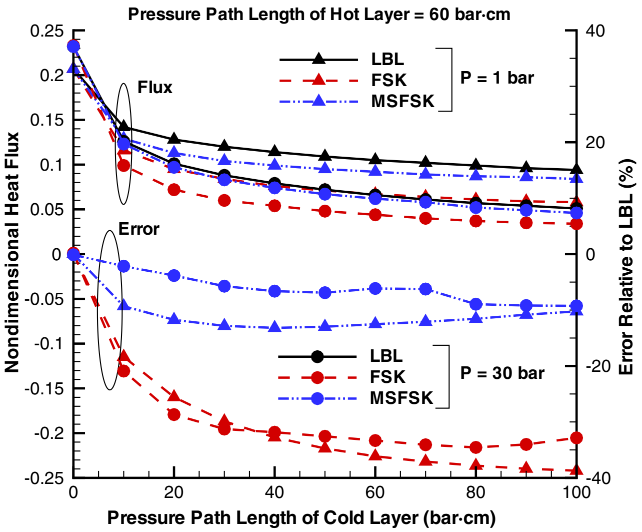

Fig. 2 Nondimensional heat flux leaving an inhomogeneous slab at various total pressures with step changes in concentration and temperature.

The k-distribution methods were investigated for a more realistic but artificial methane–air flame (from Modest and Zhang [10]) at 30 bar pressure. Temperature and concentration distributions for CO_2, H_2O, and CH_4 were obtained from the previous work of Modest and Zhang [10]. The local radiative heat source term was calculated using the LBL, FSK, and MSFSK approaches, employing the P-1 method as the RTE solver, and relative errors were determined by comparison with the LBL method as

$$\text{error}(\%) = \frac{\nabla \cdot q_{\text{LBL}} - \nabla \cdot q_{\text{FSK/MSFSK}}}{\nabla \cdot q_{\text{LBL,max}}} \times 100 \tag{6}$$

The maximum error in the local radiative heat source term is 11% using the FSK method and 2% using the MSFSK method (see Fig. 3), while their atmospheric counterparts have local maximum errors of 30% using the FSK method and 7% using the MSFSK method (see

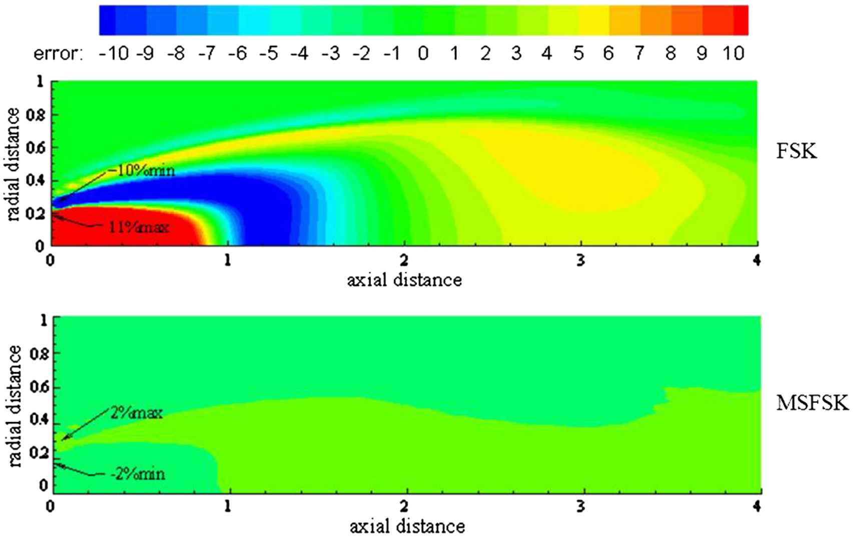

Fig. 3 Relative error for radiative heat source calculations using FSK and MSFSK methods compared to LBL method in an artificial 2-D combustion chamber at 30 bar pressure.

Pal and Modest [14]). The axial and radial distances in Fig. 3 refer to distances normalized by the total axial length and the diameter of the domain, respectively.

IV. Conclusions

The *k*-distribution methods were successfully applied to radiation calculations in participating media at high pressure. The accuracy of the underlying mixing model was tested for gas mixtures at various conditions of pressure, temperature, and mixture composition. The narrowband mixing model was found to yield excellent accuracy except at an extremely localized part of the spectrum, and this inaccuracy had no effect on the heat transfer calculations. All basic single-scale to more advanced *k*-distribution methods consistently yielded excellent accuracy when applied to one-dimensional and two-dimensional media.

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