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A k-DISTRIBUTION-BASED SPECTRAL MODULE FOR RADIATION CALCULATIONS IN MULTI-PHASE MIXTURES

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ABSTRACT

k-distribution-based approaches are promising models for radiation calculations in strongly nongray participating media. Advanced k-distribution methods were found to achieve close-to benchmark line-by-line (LBL) accuracy for strongly inhomogeneous multi-phase media accompanied by several orders of magnitude smaller computational cost. In this paper, a k-distribution-based portable spectral module is developed, incorporating several state-of-the-art k-distribution methods along with compact and high-accuracy databases of k-distributions. The module construction is flexible – the user can choose among various k-distribution methods with their relevant k-distribution databases, to carry out accurate radiation calculations. The spectral module is portable, such that it can be coupled to any flow solver code with its own grid structure, discretization scheme, and solver libraries. This open source code module is made available for free for all noncommercial purposes. This article outlines in detail the design and the use of the spectral module. The k-distribution methods included in the module are briefly described with a discussion of their advantages, disadvantages and their domain of applicability. Examples are provided for various sample radiation calculations in multi-phase mixtures using the new spectral module and the results are compared with LBL calculations.

INTRODUCTION

Radiative heat transfer is often the dominant mode of heat transfer in commercial combustion systems and atmospheric processes. The magnitude of radiative heat fluxes can have profound effects on combustion performance and on environmental impact. In commercial combustion applications erroneous prediction of gas temperature by as little as 50^oC may lead to vastly wrong prediction of its pollution characteristics. Therefore, accurate determination of radiation is necessary for correct prediction of overall heat transfer in combustion systems in order to achieve energy-optimized, economic and pollution-free performance. Traditionally, radiation in combustion systems has been treated using gray or even simpler models due to their simplicity and faster computation. Only during the past few years a number of investigators considered nongray radiation effects, using spectral models of varying levels of sophistication; all have shown a strong influence of spectral radiation in the combustion process [1–10]. Consideration of nongray thermal radiation introduces a new difficulty, as radiative properties exhibit strong and erratic variations with wavenumber for the participating species that are of interest in combustion [principally water vapor (H_2O), carbon dioxide (CO_2), and carbon monoxide (CO)].

Nongray radiation calculations in participating media can be most accurately performed using the line-by-line (LBL) approach. LBL accurately resolves the spectrum [11–15] requiring in excess of one million spectral solutions to the RTE, thus making spectral radiation calculations prohibitive (in both computational time and memory requirements) even with todays computer resources. For accurate and computationally efficient solutions of the radiative transfer equation (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 [16, 17], the absorption distribution function (ADF) method [18, 19], and the full-spectrum k-distribution (FSK) method [20]. 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 the 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. Although the FSK scheme is exact for radiative calculations in homogeneous media, its application to strongly inhomogeneous emitting–absorbing mixtures, containing both molecular gases and nongray soot particles, challenges its accuracy.

Several advancements to the k-distribution method have been proposed to address the shortcomings of the basic FSK

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scheme. To alleviate inaccuracies in inhomogeneous gas mixtures, two different approaches have been proposed, namely, the multi-scale (MS) [12] approach and the multi-group (MG) approach [21, 22]. In the multi-scale or fictitious gas approach the individual spectral lines comprising the absorption coefficient are placed into separate scales based on their temperature dependence. In the multi-group approach spectral positions, i.e., wavenumbers, are placed into several groups according to their dependence on temperature and partial pressure. The multi-group FSK (MGFSK) method has been shown to achieve great accuracy for a single gas species with inhomogeneity in temperature [12, 21, 22], whereas the multi-scale FSK (MSFSK) method can efficiently treat mixtures of absorbing gases with severe species inhomogeneity [23]. Combining the advantages of both methods, a hybrid multi-scale multi-group FSK (MSMGFSK) method has also been developed, which can accurately determine radiation from gas mixtures with extreme inhomogeneities in both temperature and concentration [24, 25]. Soot radiation constitutes an important part of radiation calculations in luminous flames. Because of the difficulties in soot modeling and because of its somewhat more benign spectral behavior, soot radiation in combustion has commonly been treated as gray [26]. Nongray soot has been investigated by Solovjov and Webb [27] using the SLW method, and by Wang *et al.*, who employed the single-scale FSK method [2]. Both these methods cannot address the species concentration inhomogeneity problem. The MSFSK method previously developed by Zhang and Modest [12] has been recently extended allowing for nongray soot in the gas mixtures with/without gray wall emission [28, 29]. However, the modified MSFSK method fails to produce accurate results in the presence of strong temperature inhomogeneities. Final advancement of the *k*-distribution concept was achieved by Pal and Modest by extending the full-spectrum-based hybrid MSMGFSK method to a narrow band-based hybrid MSMGFSK method to allow incorporation of nongray soot into the gas mixtures [30]. This narrow band-based MSMGFSK method was found to achieve close-to LBL accuracy in presence of both temperature and concentration inhomogeneities in a multiphase mixture.

FSK calculations are very accurate and time efficient provided the required full-spectrum *k*-distributions are known, which are tedious to compile from spectroscopic databases, such as HITRAN [31], HITEMP [32] and CDSD-1000 [33]. To make accurate FSK calculations feasible for general engineering purposes, preassembled FSK distribution must be available in the form of accurate and compact databases. Wang and Modest [34] have compiled a high accuracy, compact database of narrow band *k*-distributions for the most important combustion gases, from which full-spectrum *k*-distributions can be obtained efficiently for arbitrary mixtures of combustion gases, including nongray absorbing and/or scattering particles. Full-spectrum multi-group databases have been constructed by Zhang and Modest for carbon dioxide and water vapor [21, 22]. It has been reported that close-to LBL accuracy can be achieved by considering only 4 such groups, within which the assumption of a correlated absorption coefficient holds. In the multi-group databases created by Zhang and Modest [21, 22] the absorption coefficients were obtained from the HITEMP spectroscopic database. Unfortunately, it has been found that the HITEMP database is not accurate for CO_2 at temperatures higher than 1000 K [33, 35]. Recently Pal and Modest constructed more accurate and compact full-spectrum multi-group [24, 25] and narrow band multi-group databases [30] containing 4 groups for each species with spectral absorption coefficients for water vapor calculated from HITEMP 2000 [32], and for carbon dioxide from CDSD-1000 [33]. With accurate mixing models developed within the framework of advanced *k*-distribution methods in conjunction with the accurate and compact *k*-distribution databases, it is now possible to mix *k-g* distributions of multiphase species on the fly with efficient usage of memory and computational time.

In this article, an open source code *k*-distribution method-based portable spectral module, called "Spectral Radiation Calculation Software" (SRCS), has been developed. The SRCS includes all state of the art *k*-distribution methods. High-accuracy databases of *k*-distributions [25, 30, 34], together with our mixing models [12, 23, 25, 29, 30, 36], allow on-the-fly construction of FSK distributions. The module construction is flexible – the user can choose among various *k*-distribution methods with relevant *k*-distribution databases and perform accurate radiation calculations during the solution of combustion problems. The user has the choice to use the basic FSK method with a coarser grid during the initial stage of the combustion calculation and then move on to more sophisticated *k*-distribution models and finer grids during later stages of the computation. The spectral module is made portable, such that it can be coupled to any flow solver code with its own grid structure, discretization scheme, and solver libraries. Detailed module structure has been outlined in this paper including a discussion of various *k*-distribution methods with their applicability. Sample calculations were performed for a 1-D medium containing a gas–soot mixture with distributions in temperature and species concentrations using various *k*-distribution methods implemented within the SRCS. Computational time and accuracy of results obtained from different *k*-distribution methods are compared to LBL calculations.

MODULE STRUCTURE

The "Spectral Radiation Calculation Software" (SRCS) has been developed in FORTRAN-90. The schematic diagram in Fig. 1 shows the software architecture of SRCS. The various modular parts of SRCS are: 1) methods (*k*-distribution and LBL) 2) databases (*k*-distribution and LBL), 3) spectral inputs, 4) main operating module, and 5) inter-language portability module. The various modular parts of the SRCS are discussed in detail in the following sections.

Methods

The SRCS includes all state of the art *k*-distribution methods (both full-spectrum and narrow-band based) and the LBL method for spectral radiation calculations. *k*-distribution methods implemented in SRCS are summarized in tabular form with their advantages and shortcomings and shown in Table 1.

The narrow-band (NB) module, full-spectrum (FS) routines, all data retrieval modules, and line-by-line (LBL) routines are submodules under the method module. Functionality of each of the submodules is summarized in Table 2 and is described in details next.

1) LBL Submodule: Retrieves LBL absorption coefficient data from line-by-line database (only for CO_2 and H_2O) compiled by Wang and Modest [34]. This submodule is also capable to calculate absorption coefficient data from the spectroscopic databases on the fly. LBL submodule contains routines to construct *k-g* distributions (both full-spectrum and narrow-band

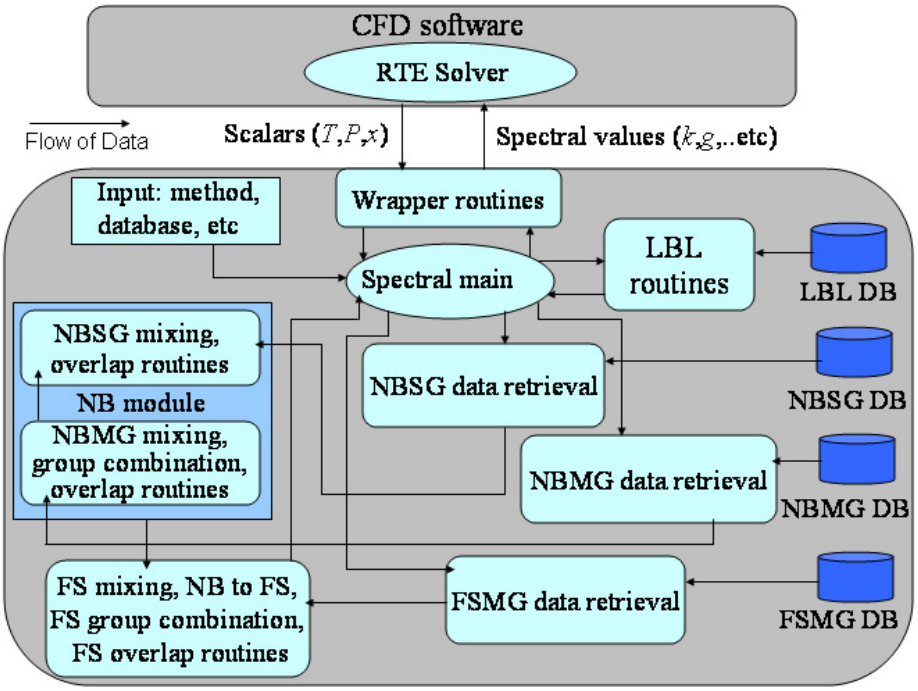

Figure 1. Software architecture diagram of SRCS

based) directly from high-resolution databases.

2) Data Retrieval Submodule: This submodule retrieves *k-g* distribution data from various *k*-distribution databases (databases discussed under database section). Depending on the scalar data (P,T,x) (state variable) information and the user's choice of *k*-distribution database, the data retrieval module opens the corresponding database and obtains the *k-g* data by interpolation. Two different data retrieval schemes have been implemented (subject to user's choice): 1) loading of the whole database into memory (computationally efficient), or 2) keeping the database files open and set a pointer to it so that information from given *(P-T-x)* grid space can be read when needed (memory efficient). Flexibility has been offered to the user in database interpolation also. The user can choose either linear or spline interpolation for any state variable (i.e., pressure, temperature, and mole-fraction) during database interpolation. The linear interpolation method is faster but can be less accurate, while spline interpolation can be more accurate, but is always more CPU intensive. A detailed discussion of database interpolation methods can be obtained from Wang and Modest [34]. The data retrieval module contains three submodules (as mentioned in Table 2) : 1) FSMG data retrieval module – to retrieve full-spectrum multi-group data from the full-spectrum multi-group database; 2) NBSG data retrieval module – to retrieve narrow-band single-group data from the narrow-band single-group database; and 3) NBMG data retrieval module – to retrieve narrow-band multi-group data from the narrow-band multi-group database.

3) Narrow-band Submodule: The narrow-band submodule is again divided into two submodules: 1) narrow-band single-group and 2) narrow-band multi-group submodules as shown in Table 2.

The narrow-band single group module contains routines for narrow-band based mixing of species (outlined by Modest and Riazzi [36]) and narrow-band based single-group overlap parameter calculations (outlined by Pal and Modest [29]). The narrow-band single-group module receives *k-g* data via the NBSG data retrieval module; performs narrow-band based mixing of *k-g* data and overlap parameter calculations and returns the narrow-band data to the FS module (shown in Fig. 1).

The narrow-band multi-group module contains routines for narrow-band based multi-group overlap parameter calculations and group combination at the narrow-band level (outlined by Pal and Modest [30]). The narrow-band multi-group module receives *k-g* data via the NBMG data retrieval module; performs narrow-band based overlap parameter calculations and returns the narrow-band data to the FS module (shown in Fig. 1).

4) Full-spectrum Submodule: The full-spectrum submodule contains two submodules: 1) full-spectrum multi-group routines, and 2) narrow-band to full-spectrum assembly routines.

The full-spectrum multi-group module contains routines for full-spectrum based multi-group overlap parameter calculations and group combination at the full-spectrum level (outlined by Pal *et al.* [25]). As shown in Fig. 1 the full-spectrum multi-group module receives *k-g* data via the FSMG data retrieval module; performs full-spectrum based overlap parameter calculations and returns the full-spectrum data to Spectral Main (the main operating module, discussed later).

The narrow-band to full-spectrum assembly module combines narrow-band single/multi-group data obtained from the NB module to full-spectrum single/multi-group data (developed by Modest and Riazzi [36]) and returns data to the Spectral Main. This module is also capable of combining groups at the full-spectrum level [21, 22] to produce single-group full-spectrum *k-g* distributions.

Databases

High-accuracy compact *k*-distribution databases are a part of SRCS. All available *k*-distribution databases are summarized in Table 3. In all these databases, the spectral absorption coefficients for water vapor were calculated from HITEMP 2000

Table 1. Advanced k-distribution methods

Method	Advantages	Shortcomings
Single scale FSK [20] (8 – 10) RTEs	Most CPU efficient; accurate for moderately inhomogeneous media	Inaccurate for strongly inhomogeneous media; problems in mixing of species
Narrow-band based single-scale FSK [36] (8 – 10) RTEs	Most CPU efficient; mixing of multi-phase species; accurate for moderately inhomogeneous media	Inaccurate for strongly inhomogeneous media
Multi-scale FSK/Fictitious gas [12, 19] $N \times (8-10)$ RTEs	Accurate for mixing and species (gas only) inhomogeneity	Inaccurate for strong temperature inhomogeneity and multi-phase mixing
Multi-group FSK [21, 22] $M \times (8-10)$ RTEs	Accurate for temperature inhomogeneity in a single gas	No mixing of species; inaccurate for concentration inhomogeneity
Narrow-band-based multi-scale FSK [23] $N \times (8-10)$ RTEs	Better accuracy for mixing of gases; potential for multi-phase mixing	Inaccurate for strong temperature inhomogeneity
Multi-scale multi-group FSK [25] $N \times M \times (8-10)$ RTEs	Accurate for general inhomogeneity problem for gas mixtures	Inaccurate for multi-phase mixing
Narrow-band-based modified multi-scale FSK [29] $N \times (8-10)$ RTEs	Accurate for multi-phase mixing and species inhomogeneity	Inaccurate for strong temperature inhomogeneity
Narrow-band-based multi-scale multi-group FSK [30] $N \times M \times (8-10)$ RTEs	Accurate for multi-phase mixing and strong inhomogeneous media	CPU expensive relative to single-scale FSK

[32], for carbon dioxide from CDSD-1000 [33], and all other species from HITRAN-2004 [37]. The narrow-band single group k-distribution databases constructed by Wang and Modest [34] have been extended to include more combustion species, such as CO, CH_4,and C_2H_4. Various values of total pressure, local gas temperature, and species mole fraction and/or Planck function

Table 2. Submodules within method module

Module	Submodule	Functionality
LBL Module		Retrieves LBL data from LBL database; constructs LBL FS and NB k-g distributions
Data Retrieval Module	FSMG Data Retrieval	k-g data from FSMG database by interpolation
	NBSG Data Retrieval	k-g data from NBSG database by interpolation
	NBMG Data Retrieval	k-g data from NBMG database by interpolation
NB Module	NBSG routines	Narrow-band based mixing and overlap parameter for single-group k-g data
	NBMG routines	Narrow-band multi-group based mixing and overlap parameter for multi-group k-g data; group combination to produce single-group k-g data
FS Module	FSMG routines	Full-spectrum based mixing and overlap parameter for multi-group k-g data; group combination to produce single-group k-g data
	NB to FS conversion	Conversion of narrow-band data from NB module to full-spectrum

Table 3. k-distribution databases

Databases	Species
Full-spectrum multi-group	CO_2 and H_2O
Narrow band single group	CO_2,H_2O,CO,CH_4,C_2H_4
Narrow band multi-group	CO_2,H_2O

temperature, for which k-g distribution data are stored, can be obtained from Wang and Modest [34]. For any given arbitrary state (P,T,x), the k-g data can be obtained from the database by interpolation (as described in the Data Retrieval Module section). Typical data retrieval time for interpolated state conditions from the FSMG database is $\approx$ 1 ms (4 full-spectrum k-g distributions), from the NBSG database $\approx$ 3 ms (248 narrow band k-g distributions), and from the NBMG database $\approx$ 6 ms (4×248 narrow band k-g distributions) using a 3.0 GHz Intel Xeon machine.

Spectral Input

SRCS has been designed to offer user flexibility. Through the spectral input module the user interacts with the core software. The spectral input module has two parts: 1) spectral input file and 2) input check submodule.

In the spectral input file the user can specify: 1) k-distribution method, 2) k-distribution database, 3) number of quadrature points for spectral integration, 4) species identifers, 5) if a multi-scale method is chosen, species identifiers for combination of species scales (optional) are chosen, otherwise each species is treated as one scale, 6) database interpolation method, and 7) whether database is to be loaded into memory (yes/no).

The input check module performs compatibility checks of the spectral input parameters specified by the user. If the input parameters are incompatible, an error message is generated and an instruction is given to the user to choose correct compatible input parameters for running applications. As an example, if the user chooses the narrow-band based modified-MSFSK method [29], as listed in Table 1, with the full-spectrum multi-group database [25], an error message is generated as the method and database are incompatible with each other. A quick suggestion for the choice of database is given to the user based on the user's choice of k-distribution method.

Main Operating Module

The Spectral Main (shown in Fig. 1) or main operating module is the central processing and handling core of the SRCS software. This main module receives scalar (P,T,x) data from the RTE solver, and reads in the spectral input data specified by the user. If all inputs are correct, it passes the information to the corresponding data retrieval module. The Spectral Main receives full-spectrum data from the FS module (the FS module obtained full-spectrum data directly from the FSMG database or narrow-band from the NB Module and assemble to full-spectrum data) and supplies the full-spectrum spectral property scalars to the RTE solver.

Inter-Language Portability Module

Since SRCS is designed to supply spectral radiation properties to a RTE solver, it should have allowance to be interfaced with any existing RTE solver. For portability of this FORTRAN-90 based software with C/C++ based RTE solvers, a module is provided at the top level for interfacing C/C++ based RTE solvers with SRCS. This interfacing is placed between the RTE solver and Spectral Main of the SRCS (since Spectral Main handles the in and outflow of data to and from SRCS). This interfacing module is shown in Fig. 1 as "wrapper routines." The module contains header files containing definitions of FORTRAN-90 functions and subroutines, which are needed for the data flow, and C/C++ based routines to map C/C++ format data to FORTRAN-90 format data. Currently, the Fortran-90 based SRCS is coupled with the C++ based *P-1* RTE solver implemented in the open source-code flow software OpenFOAM (Version 1.5) [38].

SAMPLE CALCULATIONS

Sample calculations were performed for a 1-D medium containing CO_2–H_2O–N_2 gas mixtures with soot confined between cold black walls to demonstrate the performance of the SRCS.

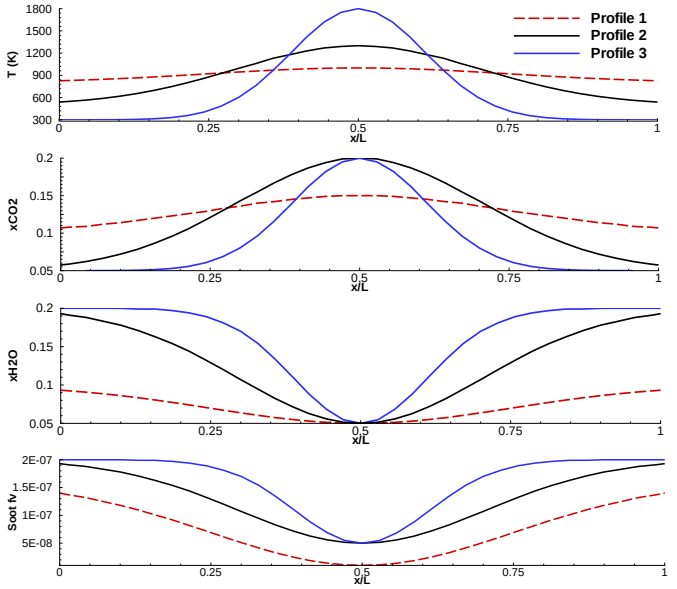

Figure 2. Temperature and mole-fraction/volume-fraction distributions of CO_2, H_2O and soot in a 1-D medium

The total pressure is kept constant at 1 bar. Gaussian distributions of temperature and concentration of each species within the medium is considered and shown in Fig. 2. As can be seen, three different scalar distribution profiles were considered. From Profile 1 to Profile 3, the local gradient of scalar distributions (i.e. temperature and species concentrations) increases. Thus Profile 1 serves a benign test case, and Profile 2 and 3 are progressively more severe test cases.

For each of these cases the local radiative source term was calculated using the LBL method, the single-scale FSK method, the modified MSFSK method, and the present narrow band-based MSMGFSK method (using 2 and 4 groups) as spectral model and finite volume based *P-1* as RTE solver. The x-direction of the 1-D medium is discretized into 40 finite volume cells. 10 Gaussian quadrature point integration over the spectral space is used for all k-distribution methods. The total number of RTEs solved for each finite volume cell is: 1.5 million for LBL, 10 for single-scale FSK, 3×10 for modified MSFSK (each species as one scale), 5×10 and 9×10 for narrow-band based MSMGFSK (each species as one scale, CO_2 and H_2O scales having 2 and 4 groups each respectively). Calculations were done in a 3.0 GHz Intel Xeon machine. CPU times for the various spectral models are typically as follows: 8920 sec (8916 sec – property acquisition and 4 sec – RTE solution) for LBL, 23 sec (22 sec – k-distribution assembly and 1 sec – RTE solution) for the single-scale FSK, 122 sec (120.5 sec – k-distribution assembly and 1.5 sec – RTE solution) for the modified-MSFSK, 216 sec (214 sec – k-distribution assembly and 2 sec – RTE solution) for the 2 group narrow-band based MSMGFSK, and 401 sec (398.5 sec – k-distribution assembly and 2.5 sec – RTE solution) for the 4 group narrow-band based MSMGFSK method. Obviously, CPU savings achieved by the k-distribution methods, while substantial, will be much greater for three-dimensional problems (when CPU time becomes dominated by the number of RTEs to be solved). Relative errors are determined by comparison with LBL as

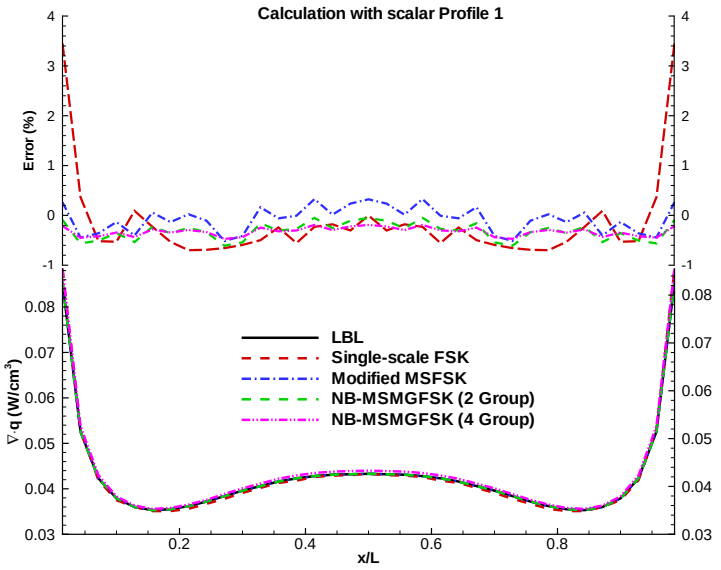

Figure 3. Local radiative heat source and relative error (compared to LBL) for heat source calculations using scalar distribution profile 1

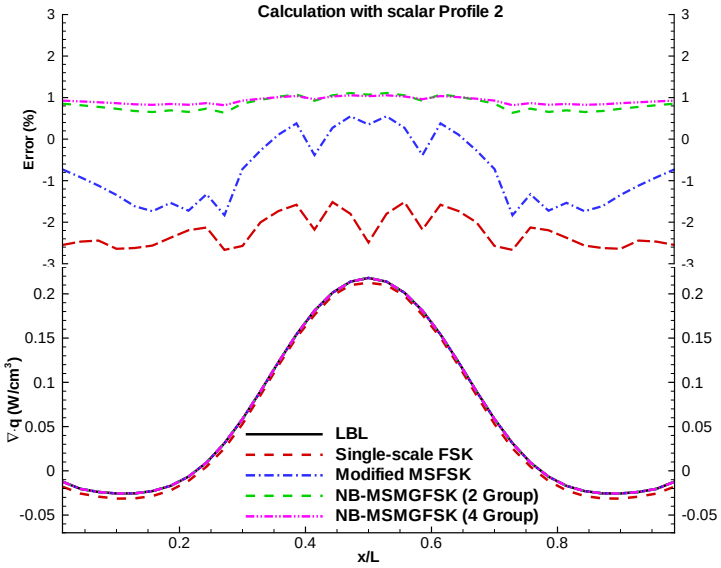

Figure 4. Local radiative heat source and relative error (compared to LBL) for heat source calculations using scalar distribution profile 2

$$\text{error}(\%) = \frac{\nabla \cdot q_{\text{LBL}} - \nabla \cdot q_{\text{FSK/MSFSK/MSMGFSK}}}{\nabla \cdot q_{\text{LBL,max}}} \times 100 \quad (1)$$

Results of radiation calculations with scalar Profile 1 are presented in Fig. 3. In this case, the maximum error of the basic single-scale FSK method incurs a maximum 3% error very close to the boundaries, otherwise remains bounded within 1%. The modified MSFSK method and both the 2 and 4 groups based MSMGFSK calculations yield better accuracy (maximum error limited to 1% for each case). For such benign scalar gradients all the k-distribution methods perform almost equally well and, hence, the basic single-scale FSK method is recommended to be used due to its low computational cost.

Results of radiation calculations with scalar Profile 2 are shown in Fig. 4. As seen from the figure, the maximum error of the basic single-scale FSK method again is only 3%. The modified MSFSK method reduces the maximum error to below 2%. Both the 2 and 4 groups based MSMGFSK calculations yield better accuracy (maximum error limited to 1% for both). It is observed that the accuracy of the 2 and 4 group based calculations are close to each other, which apparently is due to the presence of compensating errors between grouping of absorption coefficients and mixing among different absorbing species as argued by Pal and Modest [30].

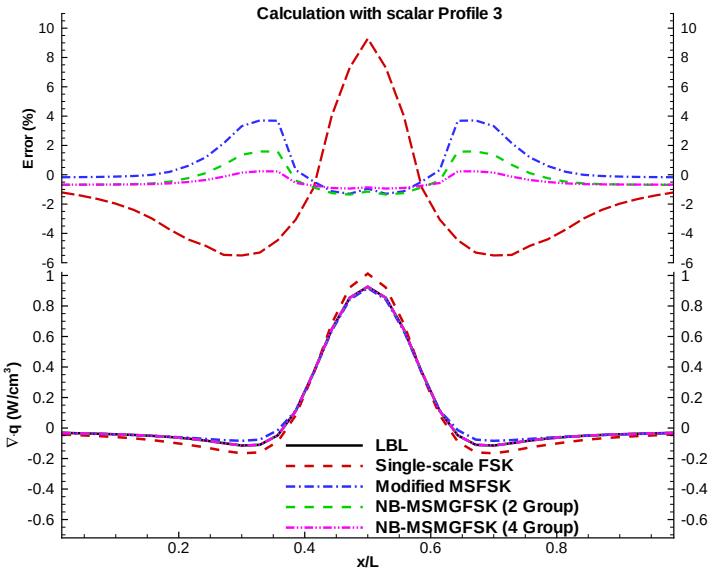

Figure 5. Local radiative heat source and relative error (compared to LBL) for heat source calculations using scalar distribution profile 3

Finally calculations were performed with scalar Profile 3 (most severe case) and results are shown in Fig. 5. It is observed here that the 2 and 4 group based MSMGFSK method have a maximum error of only 2%, whereas the single scale FSK method incurs a maximum error close to 10%, and the modified MSFSK method of 4%. For such a case the choice of the basic single-scale FSK method will lead to marginal accuracy predicting the radiative source term. If very close-to LBL accuracy is desired rather than faster computation, the user may want to choose a more advanced method, such as the narrow-band based MSMGFSK or the modified MSFSK method.

CONCLUSIONS

In this article a portable spectral module, called "Spectral Radiation Calculation Software" was developed, which includes all state-of-the art k-distribution methods and databases. The module construction is made flexible to offer the user choices of various k-distribution methods with compatible k-distribution databases. A discussion of the architecture (modules and submodules and their structures) of the SRCS has been given as well as a summary of k-distribution methods and databases implemented in SRCS. This software is designed in a modular structure for better maintenance, further development and portability (i.e., ease of interfacing with any existing flow solver). Example calculations in a 1-D medium were provided to demonstrate the performance of SRCS, for both accuracy and performance.

Guidelines have been given based on sample calculations to facilitate the choice of methods to achieve optimized computational performance and accuracy of spectral radiation calculations.

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