Radiative heat transfer calculations using full spectrum k-distribution method for benchmark test cases

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Abstract. In the present work, the full spectrum k-distribution method (FSK) has been adopted to calculate the radiative transfer in the presence of participating gaseous medium within an enclosure. The radiative properties of the medium is obtained from the HITEMP-2010 database. Further, the radiative properties have been assembled into a monotonically increasing function using the FSK. Moreover, a look-up table has been developed for these properties at different thermodynamic states and a multi-dimensional linear interpolation technique for unavailable thermodynamic states of gases. Furthermore, the FSK method is extended for mixture of gases using different mixing models such as superposition, multiplication and hybrid models. The radiation transfer equation (RTE) is solved by finite angle method to calculate the wall heat fluxes and the divergence of radiative heat flux for various test cases in the categories of homogeneous and non-homogeneous medium having different conditions of temperature and mole-fraction. The multiplication mixing model produces most accurate results among the mixture models used here. The results obtained from FSK has been validated against benchmark solution of line by line method (LBL). The FSK method has been also successfully applied to non-homogeneous gaseous medium for single gas or mixture of gases with almost LBL accuracy at extremely less computational cost.

Keywords. Non-gray radiation; line by line method; FSK look-up table; multidimensional linear interpolation; gas mixing models.

1. Introduction

Radiation heat transfer plays a major role in many engineering applications, like, combustion, rocket propulsion, stealth vehicles, ablation of re-entry vehicles etc. Neglect or inaccurate treatment of radiation may lead to significant error in the estimation of the temperature profile, species distribution, pollutant emission or thermal protection. The heat transfer due to conduction and convection can be well determined theoretically or experimentally with a reasonable amount of accuracy and economy even for complex geometries. However, the same does not imply for radiation, as calculation of radiative heat flux even for simple two-dimensional geometries can be extremely difficult due to presence of participating media such as gases and particulate matters.

Gray medium is an engineering approximation where a constant value of absorption coefficient is assumed and the spectral variation of radiative properties are neglected. It simplifies the radiative transfer calculation however, for some engineering applications like, combustion, rocket propulsion, it may lead to a significant amount of inaccuracy in predicting various quantities like flux, temperature distribution, species production etc.

Unlike solids and liquids, gases do not emit and absorb energy in a continuous manner but, they emit and absorb energies in discrete bands at resonant frequencies which give dark or bright lines on a spectrum. Further, the spectral lines get broadened and partially overlap each other due to internal collisions and the other effects. This makes spectral absorption coefficient calculation a challenging task which in turn makes the calculation of radiation heat transfer extremely difficult. The accurate calculation of absorption coefficient can be performed using some of the most popular available databases like high resolution transmission spectroscopic molecular absorption database (HITRAN) [1], carbon-dioxide spectroscopic database (CDSD) [2], high temperature spectroscopic absorption parameter (HITEMP) [3, 4] etc.

Several non-gray models evolved over time and can be classified into three different categories namely (1) Line by line, (2) Band models, (3) Global models. Line-by-line method (LBL) is the most accurate non-gray method, as it solves the RTE for each line on spectral scale. Even after
advancements in computers, LBL calculations are used only for benchmarking purposes. As radiation heat transfer is a small part of big multi-physics problems, like combustion, where it is required to solve for mass and species conservation for species transport, reaction chemistry, fluid flow, turbulence and their interactions with other modes of heat transfer coupled together, thus special consideration is needed for radiation heat transfer to reduce resource requirement as much as possible for it.

The next class of non-gray model which gained a large amount of popularity is the band model. This model does not solve RTE for each spectral line, instead splits the whole spectral scale into a number of bands. Further, development in the field of band models leads to the development of narrow band and wide band models.

The narrow band model was first developed by Malkmus and Goody [5, 6], where the actual variation of absorption coefficient is smoothed by taking an average over the narrow band. It gives good accuracy and is cheaper than LBL but it cannot be applied to non-homogeneous medium which is the biggest limitation of this method. The wide band model introduced by Edward [7] requires averaging to be done over the whole ro-vibrational band and its accuracy is even lesser than narrow band model. It considers the fact that the black body intensity does not vary significantly over the whole spectral range, thus, its correlations can be developed by integrating the narrow band over the entire spectrum.

The global models are one of the best available non-gray models in terms of accuracy and computational resource requirement, some of the most commonly used global models are weighted sum of gray gas model (WSGG), spectral line weighted sum-of-gray gases model (SLW), absorption distribution function model (ADF), full Spectrum k-distribution method (FSK). The weighted sum of gray gas model was initially developed by Hottel and Sarofim [8], as the name suggests, it relates the non-gray gas into number of gray gases having different weights and thus, solves RTE for different gray gases. Nevertheless, this method is restricted to black wall enclosures containing non-scattering medium. This model is further improved by spectral line weighted sum-of-gray gases model including non-isothermal and non-homogeneous medium by introducing cumulative distribution of absorption coefficient into weighted fractional Planck function over the entire spectrum by Dension and Webb [9]. The absorption distribution function model (ADF) [10] differs from SLW only in terms of weight considered for the gray gases. The full Spectrum k-distribution method which can be used extensively for non-homogeneous medium by correlating or scaling the absorption coefficient, developed by Modest and Zhang [11] is one of the best available non-gray radiation model and can be used for scattering media with gray walls.

This method is further improved by considering the conservation of emission [12]. It is also stated by Modest that WSGG is only a crude implementation of FSK. Global models can be used easily with any of the available RTE solvers without any modifications. Some of the most popular numerical techniques to solve RTE are spherical harmonics $P_N$ method, discrete ordinate method (DOM), discrete transfer method (DTM), finite volume method (FVM), Monte Carlo method etc.

In the present study, the calculation of non-gray radiative heat transfer has been performed for non-homogeneous and non-isothermal participating medium in an enclosure. The medium is filled with the mixture of participating gases such as $H_2O$ and $CO_2$ at different thermodynamic states of temperature and mole-fraction. The radiative properties are evaluated from HITRAN-2010 database and is reordered using full spectrum k-distribution method. Further, the FSK database (FSK look-up table) is generated to make it applicable for the non-homogeneous and non-isothermal medium by pre-calculating the properties and storing it for different thermodynamic states. An efficient scheme of interpolation has also been presented to evaluate the value of radiative properties which are not available in the look-up table. Several mixing models have also been presented to obtain k-distribution for mixture of participating gases for both homogeneous isothermal medium and non-homogeneous non-isothermal medium.

The manuscript is organised as section 2, describes the detailed mathematical models to obtain spectral absorption coefficient, full spectrum k-distribution for individual gas and gas mixtures, followed by results and discussions in section 3, and finally the present work is concluded in section 4.

2. Mathematical model

2.1 The spectral radiative transfer equation

The spectral radiative transfer equation (s-RTE) for the participating medium can be obtained by making spectral radiative energy balance for a pencil ray that passes through the medium. A ray gets attenuated due to absorption and out-scattering and augmented by emission and in-scattering. Considering all the above phenomena, the equation of radiation transfer for a monochromatic ray is given as [13, 14],

$$\frac{dI_\lambda}{ds} = \kappa_\lambda I_\lambda - \beta_\lambda I_\lambda + \frac{\sigma_m}{4\pi} \int_{4\pi} I_\lambda(\hat{s}_i) \Phi_\lambda(\hat{s}_i, \hat{s}) d\Omega_i ,$$

(1)

Above equation is subjected to wall boundary condition as below,
where, $\epsilon_w$ is the spectral wall emissivity, $I_\eta$ is the spectral intensity along $\hat{s}$, $I_{bn}$ is the Planck function, $\kappa_\eta$ is the spectral absorption coefficient, $\eta$ is the wavenumber, $\sigma_{sn}$ is the spectral scattering coefficient, $\beta_\eta$ is the spectral extinction coefficient, $\Phi_\eta$ is the spectral scattering phase function which gives the probability of ray getting scattered from one direction to other and $\Omega$ is the solid angle.

Although above (Eq. 1) considers all the phenomena of radiation, however, only absorption and emission phenomena in a gaseous medium are considered in the present work. Thus, the general RTE for above two phenomena is written as,

$$\frac{dI_\eta}{ds} = \kappa_\eta I_{bn} - \kappa_\eta I_\eta$$

(3)

However, it is subjected to same boundary condition as Eq.(2). The solution of above equation will provide the spectral intensity field in different directions. The radiative flux can be calculated from the spectral intensity field as,

$$q = \int_0^\infty q_\eta d\eta = \int_0^\infty \int_{4\pi} I_\eta |\hat{n} \cdot \hat{s}| d\Omega d\eta$$

(4)

The temperature field that is obtained by considering the contribution of all the modes of heat transfer and radiation contribution is included as the divergence of radiative heat flux which is a sink term in the energy equation. Physically, the divergence of radiative heat flux represents the net loss of radiative energy from a control volume, which is equal to the difference of radiation energy emitted and absorbed in the medium. Thus, divergence of radiative flux is given as,

$$\nabla \cdot q = \int_0^\infty \kappa_\eta \left( 4\pi I_{bn} - \int_{4\pi} I_\eta d\Omega \right) d\eta = \int_0^\infty \kappa_\eta (4\pi I_{bn} - G_\eta) d\eta$$

(5)

The s-RTE (Eq.1) is an integro-differential equation having six independent variables which includes three spatial coordinates, two angular directions and a wavenumber making it extremely difficult to solve for complex geometries. The complexity of the problem increases many-fold with the participating gases in the medium, due to the fact that the radiative properties of gases like, absorption and scattering coefficient vary abruptly with the electromagnetic spectrum containing millions of spectral lines for a single thermodynamic state. A proper estimation of these properties is important for calculation of heat transfer by radiation mode accurately.

These properties can be obtained from the knowledge of spectroscopy, however, high temperature spectroscopic absorption parameter (HITEMP) [3] is one of the most popular available database used to determine these properties precisely. It is developed and maintained by the "Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics". It contains the spectroscopic line information of species in 160 characters in ASCII format depicting different spectroscopic parameters. The short information about the species available in this database is given in table 1. The information is stored at the reference temperature of 296 K and pressure 1 atm. A calculation is required to obtain the spectroscopic information at different thermodynamic state and this is accurate for temperature up to 4000 K and pressure 80 bar.

### 2.2 Calculation of absorption coefficient from HITEMP-2010 database

The spectral absorption coefficient of participating gases like $CO_2$, $H_2O$, $CO$, $NO$ and $OH$ are calculated from HITEMP-2010 [3]. The LBL approach has been used to calculate the spectral absorption coefficient with a uniform spectral spacing of 0.01 cm$^{-1}$. The transition line intensity other than reference thermodynamic state of a species is obtained by following equation.

$$S_{if}(T) = S_{if}(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \exp\left(-c_2E/T\right)$$

$$\frac{\left[1 - \exp\left(-c_2\nu_{if}/T_{ref}\right)\right]}{\left[1 - \exp\left(-c_2\nu_{if}/T\right)\right]}$$

(6)

where $c_2$ is second radiation constant, $T_{ref}$ is the reference temperature, i.e., 296 K, $S_{if}(T)$, $\nu_{if}$ is the vacuum

### Table 1. Content of HITEMP-2010 database

| Molecule | Spectral Coverage (cm$^{-1}$) | Number of isotopologues | Number of transitions |
|----------|-------------------------------|-------------------------|----------------------|
| $H_2O$   | 0-30000                       | 6                       | 114,241,164          |
| $CO_2$   | 5-12785                       | 7                       | 11,193,608          |
| $CO$     | 0-8465                        | 6                       | 113,631             |
| $NO$     | 0-9274                        | 3                       | 115,610             |
| $OH$     | 0-19268                       | 3                       | 41,557              |
wavenumber, \( E \) is the lower state energy and \( Q(T_{\text{ref}})/Q(T) \) is the ratio of internal partition functions. These parameters are available in HITEMP database.

The collisional broadening phenomenon is used in the current study and this broadening phenomenon is applicable for temperature upto 2000 K and at or above atmospheric pressure. The absorption crosssection obtained from line intensity and this broadening phenomenon is shown below,

\[
k_g(v, T, p) = \left( \frac{S_g(T)}{\pi} \right) \left[ \frac{\gamma(p, T)}{\gamma^2(p, T) + (v - v_g^f)^2} \right],
\]

where, \( k_g \) is the monochromatic absorption coefficient and \( \gamma(p, T) \) is half width at half maximum (HWHM) at given temperature and pressure which can be calculated as

\[
\gamma(p, T) = \left( \frac{T_{\text{ref}}}{T} \right)^{n_{\text{air}}} \left( \gamma_{\text{air}}(p_{\text{ref}}, T_{\text{ref}})(p - p_{\text{ref}}) + \gamma_{\text{self}}(p_{\text{ref}}, T_{\text{ref}})p_{\text{self}} \right)
\]

\[
v_g^f = v_g + \delta(p_{\text{ref}})p;
\]

where \( n_{\text{air}} \) is temperature-dependence coefficient, \( \gamma_{\text{self}} \) is self-broadened half width, \( \gamma_{\text{air}} \) is air broadened half width, \( p_{\text{self}} \) is the partial pressure of gas, \( \delta \) is shift of line due to pressure.

Finally, the absorption coefficient is obtained as,

\[
\kappa = k_g \times N
\]

where \( N \) is number density of species which is given as

\[
N = (7.3392315 \times 10^{21}) \times \frac{p_{\text{self}}}{T}
\]

Algorithm for calculation of spectral absorption coefficient [15, 16]

1. Extract the required parameters from HITEMP-2010 database.
2. Calculate line intensity at required temperature from Eq.(6).
3. Evaluate Half width at half maxima (HWHM) using Lorentz profile.
4. Calculate the shift of line due to pressure.
5. Now create an equispaced division having spectral interval of 0.01 cm\(^{-1}\) for whole spectrum.
6. Consider the effect of transition upto a spectral distance of 20 HWHM from both the sides at a particular spectral location [17].
7. Evaluate monochromatic absorption coefficient and calculate absorption coefficient by multiplying it with molecule number density (\( N \)) of the radiating species.
8. Repeat steps 6 to 7 at all spectral location.
9. Filter the data to remove the noise.

In a general engineering system, there hardly exists a single participating gas, e.g., in combustion of any hydrocarbon fuel, three major participating gases are formed, i.e., \( CO_2 \), \( H_2O \) and \( CO \). So, it requires calculation of spectral absorption coefficient for mixture of gases [18] and it can be obtained as,

\[
\kappa_{\text{mix}} = \sum_{i=1}^{m} \kappa_{ni}
\]

where \( m \) is the number of participating gases.

At this point, one can imagine that there exists millions of transition lines and Eq. (3) needs to be solved on these millions of lines in each direction for a single thermodynamic state of gas. Furthermore, there exists many thermodynamic state of gases in any engineering applications like, combustion, plume radiation, gasification etc. Thus, it is formidable to use this method in the current form for any applications with the current state of the art computer technology. Many methods have been proposed to reduce the computational resource requirement as much as possible. The more realistic and accurate methods are FSK [11, 12] and SLW [9] methods developed for single thermodynamic state and it is further improved for many thermodynamic states that exists in a system. The FSK method for RTE calculation for a single thermodynamic state is described below.

### 2.3 Full spectrum k-distribution method

The spectral absorption coefficient obtained from HITEMP-2010 database is highly erratic in nature and attains same value multiple times. So, within a narrow band, where Planck function is essentially constant, it can be re-ordered into monotonically increasing function. This reduces the computational effort to solve RTE over few quadrature points which provides almost the same accuracy as solving RTE by LBL method. This method of re-ordering of spectral absorption coefficient is called the full spectrum \( k \)-distribution (FSK) method and is exact for homogeneous medium. The details about this method are given below.

#### 2.3.1 Homogeneous and isothermal medium

The full spectrum \( k \)-distribution which accounts the fractional Planck function between two absorption coefficients, i.e., \( \kappa \) and \( \kappa + \Delta \kappa \) as \( \Delta \kappa \to 0 \) is given as,

\[
f(T, k) = \left( \frac{1}{I_p} \right) \int_0^\infty I_{bg} \delta(k - \kappa)d\eta
\]

where \( f(T, k) \) is Planck function weighted \( k \)-distribution. The spectral absorption coefficient varies between zero to few hundreds over whole spectral range where lower values of absorption coefficients are large in number, thus, it is not advisable to have a uniform division of spectral absorption coefficient range as it does not capture lower absorption coefficient values efficiently. Therefore, division of...
absorption coefficient range should happen according to a power law distribution [19]. So, absorption coefficient selection over a range given below as,

\[ k = \left[ k_{min}^{pow} + \frac{i - 1}{N_{bin} - 1} (k_{max}^{pow} - k_{min}^{pow}) \right]^{1/pow} \]  

(14)

where, \( k_{min} \) and \( k_{max} \) are the minimum and maximum values of spectral absorption coefficients, respectively. Value of \( pow \) is taken as 0.3678 and the spectral axis is divided into 5000 bins \( (N_{bin}) \). It is further advisable to develop cumulative \( k \) distribution, i.e., \( g \) which is a smooth increasing function whose value lies from 0 to 1 and is obtained as,

\[ g(T, k) = \int_{0}^{k} f(T, k) \, dk, \]  

(15)

Finally, the reordered radiative transfer equation \((r\text{-RTE})\) for absorbing-emitting medium in \( g \) space is given as,

\[ \frac{dl_g}{ds} = k (I_b - I_g), \]  

(16)

subjected to wall boundary condition,

\[ I_{wg} = \epsilon_w a(T_w, T, g) \sigma T_w^4 \]

\[ + \frac{1 - \epsilon_w}{\pi} \int_{|\hat{n} \cdot \hat{s}| < 0} I_k \, |\hat{n} \cdot \hat{s}| \, d\Omega \quad \text{for} \quad (\hat{n} \cdot \hat{s} > 0) \]  

(17)

The detailed mathematical derivation to obtain \( r\text{-RTE} \) from \( s\text{-RTE} \) can be referred from [13, 14]. The transformed boundary condition contains a stretching function \( a(T_w, T, g) \) which can be calculated as,

\[ a(T_w, T, g) = \frac{f(T_w, k)}{f(T, k)} \frac{dg(T_w, k)}{dg(T, k)} \]  

(18)

It is the ratio of two \( k \)-distribution functions which are calculated at wall temperature and medium temperature, respectively. Further, it is the ratio of gradient of \( g \) function at wall and medium temperature. Finally, total intensity can be obtained as,

\[ I = \int_{0}^{\infty} I_{\eta} \, d\eta = \int_{0}^{\infty} I_{k} \, dk = \int_{0}^{1} I_{g} \, dg, \]  

(19)

g can also be termed as non-dimensional Planck weighted cumulative wavenumber and this transformation of RTE from \( \eta \) space to \( g \) space is called as full spectrum \( k \)-distribution method. Further, total radiative heat flux and divergence of total radiative flux in \( g \) space is given as,

\[ q = \int_{0}^{1} q_g \, dg = \int_{0}^{1} \int_{4\pi} I_k (\hat{s}) \, |\hat{n} \cdot \hat{s}| \, d\Omega \, dg, \]  

(20)

\[ \nabla \cdot q = \int_{0}^{1} k_g (4\pi I_b - G_g) \, dg, \]  

(21)

After constructing \( k \)-distribution function in \( g \) space, it is required to select quadrature points on \( k \)-distribution function over which \( r\text{-RTE} \) needs to be solved. The strategy to discretize \( k \)-distribution function is to fix quadrature points for \( g \) and corresponding \( k \) values can be obtained. Similarly non-gray stretching factor is also obtained for the same number of quadrature points [19, 20].

The \( k \)-distribution function is not a regular function, thus, the selection of quadrature points on \( g \) scale should be such that the most of the points lie on higher values of \( k \). Therefore, quadrature points on \( g \) scale can be selected as,

\[ g_n = \cos(\theta_n), \]

(22)

where,

\[ \theta_n = \left( \frac{n\pi}{(2p + 1)} \right) \quad n = 1, 2, \ldots, p \]  

(23)

where \( p \) is the number of quadrature points which can be 12, 16, 32 or any. It is necessary to have more number of \( k \) points at higher \( g \) side as higher values of absorption coefficient dominates the radiation transfer. The corresponding weights \( w \) for integral can be calculated as,

\[ w_n = \frac{4 \sin(\theta_n)}{(2p - 1)^{\frac{1}{2}}} \sum_{i=1}^{p} \frac{\sin(2t - 1) \theta_t}{(2 - 1)^{\frac{1}{2}}} \]  

(24)

Eq. (19) for total intensity can now be written as

\[ I = \int_{0}^{1} I_g \, dg = \sum_{i=1}^{p} I_g \, w_i \]  

(25)

Finally, algorithm to develop FSK distribution function as

1. Calculate spectral absorption coefficient of a gas from HITEMP-2010 database.
2. The spectral absorption \( \kappa_g \) axis is divided into large number of bins, say 5000 between \( k_{min} \) to \( k_{max} \). Eq. (14).
3. More number of bins leads to smoother \( k \)-distribution.
4. Evaluate the fractional Planck function between two \( k \) bins over whole spectrum.
5. Further, add the fractional Planck function cumulatively to get \( g \) distribution.
6. Obtain \( k \) and \( a \) values from fixed quadrature points on \( g \) scale.

2.3.2 Non-homogeneous and non-isothermal medium The FSK method is exact for homogeneous
medium. But, engineering problems are seldomly homogeneous. To apply above formulation of FSK for non-

different thermodynamic states of gases. We follow the later strategy [21, 22] to solve RTE for non-homogeneous and non-

temperatures ranging from 300 to 2000 K, and mole-fractions varying from 0 to 1. The database contains reordered absorption coefficient \( k \) and non-gray stretching factor \( a \) for 32 points. The information of data for different thermodynamic state is summarized in table 2.

After generating look-up table, an efficient scheme for interpolation has been utilized to calculate the values of uncorrelated absorption coefficients for the gases [24]. The mixture \( k \)-distribution produces a large error [23] as the spectral line information is lost while assembling \( k \)-distribution from single gas \( k \)-distribution. Nevertheless, several mathematical modelling [23, 24] have been developed to obtain mixture \( k \)-distribution from individual gas \( k \)-distribution, some of them are as following

\[ g_{\text{mix}}(k_{\text{mix}}) = \sum_{i=1}^{N_g} g_i(k_i) - (N_g - 1) \]  

where, \( P_{11} = (x_1, t_1) \), \( P_{12} = (x_1, t_2) \), \( P_{21} = (x_2, t_1) \) and \( P_{22} = (x_2, t_2) \) are the four combinations of temperature and mole-fraction, i.e., two variable interpolation.

2.4 Full spectrum \( k \)-distribution method for mixture of gases

Many engineering problems contains mixture of participating gases rather a single participating gas. To obtain the exact \( k \)-distribution for the mixture of gases, we need to calculate spectral absorption coefficient for mixture of gases Eq. (12), however this requires prior knowledge of all the thermodynamic states available in the problem. The calculation of mixture \( k \)-distribution from individual \( k \)-distribution produces a large error [23] as the spectral line information is lost while assembling \( k \)-distribution from single gas \( k \)-distribution. Nevertheless, several mathematical modelling [23, 24] have been developed to obtain mixture \( k \)-distribution from individual gas \( k \)-distribution, some of them are as following

\[ g_{\text{mix}}(k_{\text{mix}}) = \prod_{i=1}^{N_g} g_i(k_i) \]  

2.4.1 Superposition mixing model (SMM): It is based on the assumption, that the spectral lines do not overlap significantly, leading to addition of \( g \) values for mixture of gases

\[ g_{\text{mix}}(k_{\text{mix}}) = \sum_{i=1}^{N_g} g_i(k_i) - (N_g - 1) \]  

2.4.2 Multiplication mixing model (MMM) This model describes the probability of individual event, of uncorrelated absorption coefficients for the gases [24]. The mixture \( g \)-values can be obtained by multiplying \( g \)-values of individual gas.

\[ g_{\text{mix}}(k_{\text{mix}}) = \prod_{i=1}^{N_g} g_i(k_i) \]  

2.4.3 Hybrid mixing model (HMM): The SMM gives good results at higher value of absorption coefficient while the MMM gives good results at lower value of absorption coefficient [24], thus the convolution of above two is the hybrid model and is given as,

\[ g_{\text{mix}}(k_{\text{mix}}) = \sum_{i=1}^{N_g} g_i(k_i) - (N_g - 1) \]  

\[ g_{\text{mix}}(k_{\text{mix}}) = \prod_{i=1}^{N_g} g_i(k_i) \]  

Table 2. Information of data stored in FSK lookup table for different thermodynamic states

| Parameters        | Range         | Interval    | No. of points |
|-------------------|---------------|-------------|---------------|
| Pressure          | 1 bar         |             | 1             |
| Gas Temperature   | 300–2000 K    | Every 100 K | 18            |
| Mole fraction of CO\(_2\) | 0–0.1 | Every 0.05  | 7             |
|                   | 0.25–1        | Every 0.25  |               |
| Mole fraction of H\(_2\)O | 0–0.05 | Every 0.01  | 13            |
|                   | 0.1–0.2       | Every 0.05  |               |
|                   | 0.25–1        | Every 0.25  |               |
where, $g_{sup}(k_{mix})$ and $g_{mult}(k_{mix})$ is the mixture $g$ obtained from SMM and MMM respectively.

### 2.5 Numerical solution technique of RTE - Finite Angle Method (FAM)

The finite angle method for RTE uses [13] same grid for spatial discretization as flow equations to resolve the spatial gradient and also requires additional angular discretization to resolve the directional nature of RTE. It evaluates exact solid angle using integral making it analogous to evaluation of area and volume used in CFD problems. This method conserves the radiative flux without any loss in radiation energy. The detailed formulation has been adopted from [25, 26].

Integrating the left hand side term of RTE (Eq. 1) over the volume element $\Delta V$ as shown in figure 1 and applying Gauss divergence theorem leads to,

$$\int_{\Delta V} \frac{\partial I_\eta}{\partial S} dV = \int_{\Delta V} \hat{s} \cdot \nabla I_\eta dV = \int_{\Delta V} \nabla \cdot (\hat{s} I_\eta) dV = \int_{\Delta \Gamma} I_\eta \hat{s} \cdot \hat{n} d\Gamma,$$

where $\Delta \Gamma$ is the area of a element of the surface and $\hat{n}$ is the outward surface normal. Finally integrating RTE (Eq. 1) over the volume element $\Delta V$ and solid angle $\Delta \Omega$, (see figures 1 and 2) gives,

$$\int_{\Delta \Omega} \int_{\Delta \Gamma} I_\eta \hat{s} \cdot \hat{n} d\Gamma d\Omega = \int_{\Delta \Omega} \int_{\Delta V} (-\beta_\eta I_\eta + S_\eta) dV d\Omega,$$

The left hand side of the above equation represents the outward and inward of radiant energy through the control surfaces and right hand represents the augmentation and attenuation of energy within the control volume. Intensity is stored at the centroid of control volume and its value is assumed to be constant over any control volume. The above equation can be simplified as,

$$\sum_f I_{\eta f} \Gamma_f D_\beta = (-\beta I_{\eta p} + S_{\eta p}) \Delta V \Delta \Omega,$$

where,

$$S_{\eta p} = \kappa I_{\eta p} + \frac{\sigma_s}{4\pi} \sum_i I_i(\hat{s}_i) \phi_\eta(\hat{s}_i, \hat{s}) d\Omega,$$

and $D_\beta$ is the directional weight.

**Figure 1.** Pictorial representation of (a) Spatial discretization to resolve the gradient (b) Angular discretization to set the direction

**Figure 2.** Spectral absorption coefficient of pure $H_2O$ at 1000 K temperature and 1 bar pressure.
2. Initialize the intensity field.

Expanding equation (33) gives,

\[
\Gamma e_{gfi} D_{ei} + \Gamma w_{gwi} D_{wi} + \Gamma n_{gni} D_{ni} \\
+ \Gamma s_{gni} D_{si} + \Gamma r_{gni} D_{ri} + \Gamma b_{gni} D_{bi} \\
= ( - \beta I_{gni} + S_{gP}) \Delta V \Delta \Omega_i
\]

where, the face index \( f = e, w, n, s, t, b \) indicates east, west, north, south, top and bottom faces, respectively, \( P \) indicates the cell centroid and \( i \) represents direction.

Now \( D_{fi} \) can be expanded as,

\[
D_{fi} = n_x \left( \cos \phi_i \sin \left( \frac{\Delta \phi_i}{2} \right) \left[ \Delta \theta_i - \cos 2 \theta_i \sin (\Delta \theta_i) \right] \right) \\
+ n_y \left( \sin \phi_i \sin \left( \frac{\Delta \phi_i}{2} \right) \left[ \Delta \theta_i - \cos 2 \theta_i \sin (\Delta \theta_i) \right] \right) \\
+ n_z (\Delta \phi_i \sin \theta_i \cos \theta_i \sin (\Delta \theta_i))
\]

and

\[
\Delta \Omega_i = 2 \Delta \phi_i \sin \theta_i \sin \left( \frac{\Delta \theta_i}{2} \right)
\]

Eq. (33) contains both cell centroid and face center values of intensity. The relation between both of them is given as,

\[
I_{gni} = \alpha I_{gni} + (1 - \alpha) I_{gni,bhi}
\]

where, \( nb \) refers to the centroid value of neighbouring cell and \( \alpha \) is weight and depends on the numerical scheme used to solve RTE.

Intensity at cell centroid \( P \) is obtained for applying step scheme \( (\alpha = 1) \) in two dimensional geometry for a ray going from west to east as given below,

\[
I_{gPi} = \frac{\Delta y D_{fix} I_{gni} + \Delta x D_{fix} I_{gni} + S_{gPi} \Delta V \Delta \Omega_i}{\Delta y D_{fix} + \Delta x D_{fix} + \beta_P \Delta V \Delta \Omega_i}
\]

The step scheme assigns upstream nodal intensity to downstream node. The above calculated intensity is iterated until convergence criteria is reached, i.e.,

\[
\sum_i \left| I_{gni,new} - I_{gni,old} \right| \sum_i I_{gni,new} < 10^{-6}
\]

2.5.1 Algorithm to solve RTE

1. Calculate \( D_{fi} \) for all the cells and directions.
2. Initialize the intensity field.

3. Loop over all the directions starting from \( D_{fix} > 0 \) and \( D_{fix} > 0 \) for all the cells.
4. Iterate the solution and compute residual.
5. Repeat 3 and 4 till the desired convergence criteria is matched.

2.6 Estimation of error

The FSK solution method is compared with the LBL solution and error is estimated in FSK solution as below.

**Error in radiative flux**

\[
\%error_i = \frac{q_{ni}(LBL) - q_{ni}(FSK)}{q_{ni}(LBL)} \times 100 \tag{42}
\]

**Error in divergence of radiative heat flux**

\[
\%error_i = \frac{\nabla \cdot q_{ni}(LBL) - \nabla \cdot q_{ni}(FSK)}{\nabla \cdot q_{ni}(LBL)} \times 100 \tag{43}
\]

Further, the errors are quantified in terms of root mean square (RMS) and is defined as below:

\[
RMS_{error} = \sqrt{\frac{\sum_i \text{error}_i^2}{N}} \tag{44}
\]

3. Results and discussions

The above procedures have been employed to calculate the spectral absorption coefficients of individual \( H_2O \) and \( CO_2 \) gas and mixture of these gases. Further, the results of radiative transfer equation with FSK for single thermodynamic state and many thermodynamic states have been present and computational time and associated errors with respect to benchmark solutions are reported in the following sections.

3.1 Spectral absorption coefficient of \( H_2O \) and \( CO_2 \) gases

The spectral absorption coefficients of individual \( H_2O \) and \( CO_2 \) gases have been calculated at 1 bar pressure for 1 mole fraction for a gas column, by LBL approach from HITEMP-2010 database and are depicted in figures 2 and 3, respectively. The absorption of radiation energy occurs in three distinct spectral bands for \( H_2O \) which correspond to 6.3 \( \mu m \), 2.7 \( \mu m \) and 1.8 \( \mu m \) bands. The 6.3 \( \mu m \) band is called strong fundamental band, 2.7 \( \mu m \) is first overtone band and 1.8\( \mu m \) is second overtone band. Similarly, \( CO_2 \) absorbs the radiation in four distinct bands, which correspond to 2\( \mu m \),
The 4.3 \text{ \mu m} band is the fundamental band. The \textit{H}_2\text{O} and \textit{CO}_2 act as transparent gases for rest of the spectrum. The description of these bands for \textit{H}_2\text{O} and \textit{CO}_2 gases is shown in table 3. The spectral absorption coefficients for \textit{H}_2\text{O} and \textit{CO}_2 on the log scale are shown in figures 4 and 5, respectively.

### 3.2 FSK distribution of individual \textit{H}_2\text{O} and \textit{CO}_2 gases

The spectral absorption coefficient as calculated above is re-ordered using FSK method into smooth $k$ vs $\eta$ distribution for pure \textit{H}_2\text{O} and \textit{CO}_2 gases at 1000 K and 1 bar for single thermodynamic state of gas distributions. The $k$-distribution obtained by FSK method for both the gases is shown in figure 6 and these distributions are monotonically increasing function. Similarly, the stretching function for $T_w = 500$ and 1500, and $T_g = 1000$ for \textit{H}_2\text{O} and \textit{CO}_2 gas is shown in figure 7. This distribution is quite erratic and a should be selected carefully in-order to obtain correct solution of RTE.

### 3.3 Solution of RTE for homogeneous and isothermal medium

#### 3.3.1 Case 1

The non-dimensional radiative heat flux at the bottom wall and the divergence of radiative heat flux along the horizontal line at mid height are calculated by solving RTE using FSK for different set of quadrature points for homogeneous and isothermal condition of a gas inside a square cavity of unit dimension. The cavity is filled

| Species | Band (\text{\mu m}) | Band Description | Wavenumber Range (cm$^{-1}$) |
|---------|----------------|-----------------|-------------------------------|
| \textit{H}_2\text{O} | 6.3 | Strongest band | 1000–2100 |
| | 2.7 | Strong overtone band | 3000–4300 |
| | 1.8 | Combination band | 4800–5800 |
| \textit{CO}_2 | 15 | Fundamental band | 400–1200 |
| | 4.3 | Head-forming band | 1900–2600 |
| | 2.7 | Combination band | 3200–4000 |
| | 2.0 | Overtone band | 4600–5400 |
with pure CO$_2$ at 1000 K temperature and 1 bar pressure and the walls of the cavity are black and cold. The results obtained using FSK are compared against LBL as shown in figures 8 and 9. The non-dimensional flux and the divergence of radiative heat flux calculated with FSK almost match with 16 and above quadrature points with the results of LBL method. There is a little inaccuracy for FSK with 12 points with errors approximately 0.8% and 4% in non-dimensional flux and divergence of radiative flux, respectively, which eventually vanishes by increasing number of quadrature points. Moreover, there is drastic reduction in computational time required to solve RTE, i.e., around 28,000 times for FSK with maximum number of quadrature points ($p=64$) which is shown in table 4, along with the root mean square values of error in flux and divergence of flux.

3.3.2 Case 2 The above case is slightly modified by maintaining all the walls at 500 K and the rest conditions are kept same as in case 1. The stretching function is also required to calculate in this problem, as walls are at some temperature other than medium temperature. The non-
dimensional radiative heat flux at the bottom wall and the divergence of radiative heat flux along the horizontal line at mid height is shown in figures 10 and 11, respectively, along with the error distribution in different quadrature points. The 12 point quadrature point produces approximately 2.1% and 2.4% errors in the non-dimensional heat flux and non-dimensional divergence heat flux, respectively. These errors reduce drastically in increase in quadrature points. The computational time required to solve RTE and also the RMS of error for both radiative heat flux and divergence of radiative heat flux are shown in table 5.

### Table 4. Computational time required for the solution of RTE by different methods and quadrature points on 3.4 GHz i7 4th generation CPU along with RMS of error for radiative flux and divergence of radiative heat flux for Case 1

| Method | CPU Time (s) | RMS of Error in Flux (%) | RMS of Error in $\nabla \cdot q_r$ (%) |
|--------|--------------|--------------------------|----------------------------------|
| LBL    | 5592         |                          | 2.41                             |
| FSK-12 | 0.039        | 0.81                     | 2.41                             |
| FSK-16 | 0.052        | 0.38                     | 1.27                             |
| FSK-32 | 0.09         | 0.3                      | 0.34                             |
| FSK-64 | 0.2          | 0.3                      | 0.28                             |

### Figure 10. Non-dimensional radiative heat flux on the bottom wall along with the error distribution with different quadrature points for Case 2

### Figure 11. Divergence of radiative heat flux along the horizontal line at the mid height of the cavity along with the error distribution with different quadrature points for Case 2

3.3.3 Case 3 Finally, the above case is made more realistic by keeping temperature at one wall as 1500K, other walls are maintained at 500 K and the rest conditions are kept same as that of case 1. The non-dimensional radiative heat flux at the bottom wall and the divergence of radiative heat flux along the horizontal line at mid height are shown in figures 12 and 13, respectively. The computational time required to solve RTE is shown in Table 6 along with RMS of errors. This case takes slightly more computational time compared with other two cases, this is due to calculation of stretching function for two different temperatures and solving RTE with two stretching functions.

### Table 5. Computational time required for the solution of RTE by different methods and quadrature points on 3.4 GHz i7 4th generation CPU along with RMS error for radiative flux and divergence of radiative heat flux for Case 2

| Method | CPU Time (s) | RMS of Error in Flux (%) | RMS of Error in $\nabla \cdot q_r$ (%) |
|--------|--------------|--------------------------|----------------------------------|
| LBL    | 5657         |                          | 2.41                             |
| FSK-12 | 0.041        | 2.13                     | 2.41                             |
| FSK-16 | 0.053        | 0.14                     | 1.07                             |
| FSK-32 | 0.11         | 0.28                     | 0.44                             |
| FSK-64 | 0.23         | 0.11                     | 0.37                             |
3.4 Solution of RTE for non-homogeneous and non-isothermal medium

The non-homogeneous and non-isothermal domain can be split into regions of homogeneous and isothermal medium and the properties of each region are taken from the look-up table for the available thermodynamic states and can be interpolated using multi-dimensional linear interpolation for unavailable thermodynamic states. Accuracy of RTE solution using multi-dimensional interpolation technique have been tested for three different test cases presented below.

3.4.1 Non-homogeneous and isothermal medium

The computational domain used in this case contains CO₂ and H₂O gases at different concentrations but at fixed temperature of 1000 K. The non-homogeneous domain is trifurcated into the homogeneous regions as shown in figure 14. The left side of the domain contains 25% CO₂ and 75% H₂O, middle part contains 50% CO₂ and 50% H₂O and the right side contains 75% CO₂ and 25% H₂O. The walls of the cavity are black and cold. The radiative property of end regions is available in mixture FSK look-up table and the mid section is interpolated using a linear interpolation. The $k$-distribution obtained by interpolation is matching very well with the $k$-distribution where it is also made available for middle part as shown in the figure 15, however the non-dimensional radiative heat flux obtained from interpolation matches very well with exact FSK with maximum 0.25% error in flux as shown in figure 16.

3.4.2 Homogeneous and non-isothermal medium

The computational domain used in this case contains 50% CO₂ and 50% H₂O at different temperatures. The non-isothermal domain is trifurcated into isothermal zones as in previous cases. The left, middle and the right regions of the domain are maintained at the temperature of 1000 K, 1100 K and 1200 K respectively. The walls of the cavity are black and cold. The property of the mid section is interpolated using a linear interpolation from the FSK look-up table. The $k$-distribution match very well with exact FSK as shown in figure 17, the non-dimensional radiative heat flux obtained from interpolation matches very well with exact FSK with nearly 0.2% maximum error in flux as shown in figure 18.

3.4.3 Non-homogeneous and non-isothermal medium

The computational domain used in this case contains CO₂ and H₂O at different concentrations and temperatures. Again, the non-homogeneous and non-isothermal domain is trifurcated into homogeneous and isothermal zones as in previous cases. The left side of the domain contains 25% CO₂ and 75% H₂O at 1000 K, middle part contains 50% CO₂ and 50% H₂O at 1100 K and the right side contains 75% CO₂ and 25% H₂O at 1200 K. The walls of the cavity are black and cold. The property of the mid section is interpolated using a bi-linear interpolation from the FSK look-up table. The $k$-distribution curve by interpolation method is compared as shown in figure 19 with the exact FSK where $k$-distribution of middle portion is also generated from spectral data and these curves overlap each other, the non-dimensional radiative heat flux obtained from interpolation matches very well with exact
Table 6. Computational time required for the solution of RTE by different methods and quadrature points on 3.4 GHz i7 4th generation CPU along with RSME for radiative flux and divergence of radiative heat flux for Case 3

| Method  | CPU Time (s) | RMS of Error in Flux (%) | RMS of Error in $\nabla \cdot q_r (\%)$ |
|---------|--------------|---------------------------|--------------------------------------|
| LBL     | 5705         |                           |                                      |
| FSK-12  | 0.044        | 0.17                      | 2.33                                 |
| FSK-16  | 0.059        | 0.016                     | 1.71                                 |
| FSK-32  | 0.12         | 0.006                     | 1.30                                 |
| FSK-64  | 0.25         | 0.037                     | 1.31                                 |

Figure 14. The trifurcated geometry of unit dimension square cavity

Figure 15. Comparison of interpolated $k$-distribution obtained for middle section from FSK look-up table and exact FSK

Figure 16. Non-dimensional radiative heat flux at the bottom wall containing non-homogeneous and isothermal medium along with distribution of error

FSK with maximum error of 0.15% in flux as shown in figure 20.

3.5 Solution of RTE for mixture of gases

The solution of RTE for the mixture of gases in the previous section have been obtained by constructing the $k$-distribution for mixture spectral absorption coefficients. However, this is not always possible, here, we are evaluating the performance of three different mixing models namely, superposition mixing model (SMM), Multiplication mixing model (MMM) and Hybrid mixing model (HMM) which use the $k$-distribution of individual gas, in the following sections.

3.5.1 Homogeneous and isothermal medium  A unit dimension square cavity whose walls are black and cold contains mixture of 50% $H_2O$ and 50% $CO_2$ at 1000 K and 1 atm pressure. Figure 21 shows spectral absorption coefficient of individual $CO_2$ and $H_2O$ gases
where significant overlapping on the spectral scale is seen and corresponding FSK obtained from different mixing models is shown in figure 22. The $k$-distribution assembled by spectral addition method (SAM) is the most accurate technique and used for benchmarking of other models. It can be seen that superposition mixing model (SMM) deviates a lot from SAM at lower $g$-values because of significant overlap of spectral lines at lower absorption coefficient values. At higher $g$-values, i.e., $g > 0.9$, SMM overlaps with SAM. For multiplication mixing model (MMM) the trend is reverse when compared to SMM. The $k$-distribution profile by hybrid mixing model (HMM) is between FSK-SMM and FSK-SMM.

The non-dimensional radiative heat flux at the bottom wall and the divergence of radiative heat flux along the horizontal line at mid height are shown in figures 23 and 24 respectively, along with the associated errors in different models. The FSK with SAM is found to be most accurate when compared to LBL method. FSK-MMM gives good
results when compared with FSK-SAM with maximum error of 1%, FSK-SMM is least accurate with maximum error of approx 20% and the accuracy of FSK-HMM lies in between FSK-SMM and FSK-MMM. The RMS values of these errors are shown in table 7.

3.5.2 Non-homogeneous and non-isothermal medium A unit dimension square cavity has been bifurcated into two regions whose left part contains 25% CO₂ and 75% H₂O at 1000 K and right part contains 75% CO₂ and 25% H₂O at 1200 K and 1 atm pressure. The walls of the cavity are cold and black. Figures 25 and 26 shows the non-dimensional radiative heat flux at the bottom wall and the divergence of radiative heat flux along the horizontal line at the mid height of the cavity, respectively along with the distribution of associated errors in different models. Among all the mixing models,
MMM and HMM almost give good accuracy in comparison to SAM with maximum error of 2.9% and least accuracy achieved by SMM with the maximum error of 7%. The RMS values of these errors are tabulated in Table 8.

4. Conclusion

The non-gray radiative properties of participating gases namely, CO₂ and H₂O have been calculated from the HITEMP-2010 database and line-by-line (LBL) calculation of radiative transfer equation has been performed to obtain the radiative heat flux at the bottom wall of the cavity and the divergence of radiative flux at the horizontal line at the mid height of the cavity. This solution has been used for the benchmarking the methods of full spectrum k-distribution method (FSK) for homogeneous isothermal medium and non-homogeneous non-isothermal medium, and also for the single gas and mixture of gases. The FSK method is almost exact and highly efficient for single gas and homogeneous isothermal medium. It drastically reduces the computational time required to solve RTE, i.e., around 0.6 million times in comparison to LBL method. This method is further extended to non-homogeneous and non-isothermal medium by developing the FSK look-up table for radiative properties. An efficient multidimensional linear interpolation method is also proposed for non-available data in the FSK look-up table. Furthermore, some gas mixing methods namely SMM, MMM, HMM have been explored for the calculation of radiative heat transfer for the mixture of gases from the k-distribution of single gas and the radiative transfer calculation have been performed in a cavity. The accuracy of these mixing models are almost same in comparison to FSK for mixture of gases. These models have reduced the computational resource requirements drastically with almost same accuracy of LBL method, thus can be used with other models of fluid flow and heat transfer for the applications of combustion, plume radiation and gasifier etc.

List of symbols

\( G \)  Irradiation
\( I_\eta \)  Spectral intensity
Planck function

Number density of species

Number of participating gases

Partition function

Line intensity

Reference temperature

Stretching function

Fractional Planck function

cumulative $k$-distribution

Absorption crossection

Number of quadrature points

Self pressure of gas

Radiative heat flux

Direction vector

weight for quadrature integration

Spectral extinction coefficient

Line shift

Spectral emissivity of the wall

Wavenumber

Half width at half maximum

Air broadened half width

Self broadened half width

Spectral absorption coefficient

Divergence of radiative heat flux

Vacuum wavenumber

Solid angle

Spectral scattering phase function

Spectral scattering coefficient

Wavenumber

gas

transition from upper state $f$ to lower state $i$

reference

wall

air

self

Spherical harmonics method

Absorption distribution function

Carbon-dioxide spectroscopic database

Discrete ordinate method

Discrete transfer model

Full spectrum $k$-distribution method

Finite volume method

High temperature spectroscopic absorption parameter

High resolution transmission spectroscopic molecular absorption database

Hybrid mixing model

Half width at half maximum

Line-by-line

Multiplication mixing model

Radiation transfer equation

Spectral addition method

Spectral line weighted sum-of-gray gases model

Superposition mixing model

Weighted sum-of-gray gas model

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