Radiative heat transfer calculation for mixture of gases using full spectrum k-distribution method

Kamal Khemani and Pradeep Kumar
Numerical Experiment Laboratory (Radiation & Fluid Flow Physics)
Indian Institute of Technology Mandi, Himachal Pradesh, 175075, India
E-mail: pradeepkumar@iitmandi.ac.in

Abstract. The full spectrum $k$-distribution method is used to obtain radiative heat flux and divergence of radiative heat flux for two test cases, containing mixture of $CO_2$ and $H_2O$ at different concentration and temperature keeping pressure constant. The $k$-distribution for mixture of gases is obtained from individual gas $k$-distribution using three different mixing models, viz., superposition, multiplication and hybrid model. Further, the radiative transfer equation (RTE) is solved by the finite volume discrete ordinate method (FVDOM) to obtain the radiative flux and the radiation source term. The results obtained were compared with the FSK from spectral addition and LBL method. The multiplication mixing model provides better accuracy compared to other mixing models considered in the present study.

1. Introduction
Heat transfer due to radiation plays a major role in many engineering applications, like combustion, rocket propulsion etc. Negligence or inaccurate treatment of radiation may lead to significant error in the estimation of temperature profile, species distribution, pollutant emission or thermal protection. Therefore, it requires accurate modelling of radiation and its properties for proper estimation of above parameters. Radiation properties like absorption and scattering coefficient for participating gases like $CO_2$, $H_2O$ and particles can be obtained accurately from high temperature molecular spectroscopic database (HITEMP) [1]. The nature of absorption coefficient is highly erratic as it contains millions of spectral lines for a particular thermodynamic state. Spectral integration of RTE over these million lines requires tremendous amount of computation resource. For a general combustion system, many thermodynamic state exists, which leads to change in spectral absorption coefficient drastically. Modest and Zhang [2] developed a new class of method namely, full spectrum correlated $k$-distribution method (FSCK) which reorders the erratic absorption coefficient into smooth monotonic function, thus reduces the computational effort required to solve spectral radiative transfer equation (s-RTE). FSK is exact for homogeneous and isothermal medium. Several other non-gray models also developed with time such as spectral line weighted (SLW) [3], weighted sum of gray gas model (WSGG) [4], absorption distribution function (ADF) [5] etc. In a general combustion scenario where multiple participating gases are present, major contribution for radiation lies from $CO_2$, $H_2O$ and $CO$. It will therefore require $k$-distribution, to perform radiation transfer calculation for mixture of gases at different thermodynamic states. This can be done in two ways, either add the spectral absorption coefficient and make a $k$-distribution lookup table [6] or make a $k$-distribution lookup table for individual gas and apply mixing models to get mixture $k$-distribution [7, 8]. The later approach is convenient and is used in the current study.
The manuscript is organised as methodology in section 2 followed by results and discussions, and finally present work is concluded in section 4.

2. Methodology

The full spectrum $k$-distribution method re-orders the oscillatory absorption coefficient into monotonically increasing order and correspondingly, the redistributed RTE (r-RTE) is obtained by multiplying $\delta(k - \kappa_{\eta})/f(T,k)$ to s-RTE as,

$$\frac{dI_g}{ds} = k(I_b - I_g)$$

(1)

where, $f(T,k)$ is Planck function weighted $k$-distribution function and $g$ is cumulative $k$-distribution

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

(2)

$$g(T) = \int_0^k f(T,k)dk$$

(3)

The re-ordered absorption coefficient can be obtained by the following power law

$$k_i = \left[k_{a_{\text{min}}} + \frac{i - 1}{N - 1}(k_{a_{\text{max}}} - k_{a_{\text{min}}})\right]^{1/a}$$

(4)

where index $a$ is taken as 0.3678, $k_{a_{\text{min}}}$ and $k_{a_{\text{max}}}$ are the minimum and the maximum absorption coefficient available at any thermodynamic state, $N$ is number of intervals.

While performing $k$-distribution spectral information is lost, thus summing up the absorption coefficients of individual gases in $k$-distribution domain leads to significant error. Whereas spectral addition of absorption coefficients (SAM) and then re-ordering provides accurate results, but it is difficult to have prior information of all the thermodynamic states in any engineering system. Thus the mixing models are necessary for accurate calculation of r-RTE for mixture of gases. Three mixing models are given below as

2.1. Superposition Mixing Model (SMM):

$g_{\text{mix}}$ can be obtained from summation of $g$-values of individual participating gas with the assumption that spectral lines of the gases do not overlap significantly.

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

(5)

where, $g_i$ is the $g$-distribution of individual gas and $N_g$ is the number of participating gases.

2.2. Multiplication Mixing Model (MMM):

$g_{\text{mix}}$ can be obtained from multiplication of $g$-values of individual participating gases. It depicts the probability of individual events [7], for the assumption of uncorrelated absorption coefficients,

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

(6)
\( g_i \) is the \( g \)-distribution of individual gas and \( N_g \) is the number of participating gases.

2.3. Hybrid Mixing Model (HMM):

The superposition model provides good results at higher value of absorption coefficient while the multiplication model provides good results at lower value of absorption coefficient [7], thus the convolution of above two is the hybrid model and is given as,

\[
g_{\text{mix}}(k_{\text{mix}}) = \left[ g_{\text{sup}}(k_{\text{mix}}) \ast \log\left(\frac{k_{\text{mix}}}{k_{\text{max}}}\right) + g_{\text{mult}}(k_{\text{mix}}) \ast \log\left(\frac{k_{\text{min}}}{k_{\text{mix}}}\right) \right] / \log\left(\frac{k_{\text{max}}}{k_{\text{min}}}\right)
\]

where, \( g_{\text{sup}}(k_{\text{mix}}) \) and \( g_{\text{mult}}(k_{\text{mix}}) \) is the mixture obtained from superposition and multiplication model respectively.

3. Results and Discussions

3.1. Homogeneous and Isothermal Medium:

The above models have been first tested for a square cavity whose walls are cold and black contains mixture of 50% CO\(_2\) and 50% H\(_2\)O at 1000 K. Figure 1 (a) shows the significant overlap of spectral absorption coefficients between wavenumber 0-100000 m\(^{-1}\) and 200000-400000 m\(^{-1}\). Corresponding full spectrum \( k \)-distribution for mixture of gases is depicted in Figure 1 (b) obtained from different methods. FSK with spectral addition method (SAM) is the most accurate technique to obtain mixture FSK. The superposition mixing model (SMM) deviates from FSK-SAM at lower \( g \)-values because of significant overlap of spectral lines at lower absorption coefficient values however, it overlaps with SAM at higher \( g \)-values i.e., \( g > 0.9 \). For multiplication mixing model (MMM) the trend is reverse when compared to SMM. The value of \( k \)-distribution obtained from hybrid mixing model (HMM) is between FSK-SMM and FSK-MMM.

Further, the RTE is solved by FVDOM to obtain the radiative heat flux and divergence of radiative heat flux. Figure 2 (a) shows the non-dimensional radiative heat flux and Figure 2 (b) shows the divergence of radiative heat flux in the horizontal direction at \( y = 0.5 \). FSK with SAM is exact when compared to LBL. FSK-MMM gives good accuracy when compared with FSK-SAM, with maximum error of 0.6%.

![Figure 1](image1.png)

![Figure 2](image2.png)

**Figure 1.** (a) Absorption coefficient of 50% CO\(_2\) and 50% H\(_2\)O at 1000 K (b) Comparison of \( k \)-distribution obtained from different mixing models
FSK-SMM is least accurate with maximum error of 12% and FSK-HMM lies in between FSK-SMM and FSK-MMM with the maximum error of 6%.

3.2. Non-Homogeneous and Non-Isothermal Medium:
The above square cavity has been bifurcated whose left part contains 25% $CO_2$ and 75% $H_2O$ at 1000 K and right part contains 75% $CO_2$ and 25% $H_2O$ at 1200 K. The radiative transfer calculations were performed to obtain the radiative heat flux and divergence of radiative heat flux by FVDOM method.

Figure 3 (a) and 3 (b) shows non-dimensional radiative heat flux at the bottom wall and divergence of radiative heat flux in the horizontal direction at $y = 0.5$. Among all the mixing models, FSK-MMM gives good accuracy after FSK-SAM followed by FSK-HMM and FSK-SMM. Maximum error for FSK-MMM is 2%, for HMM it is 2.5% and 4% for SMM in comparison to SAM.

![Figure 2. (a) Non-dimensional radiative heat flux at bottom wall (b) Divergence of radiative flux in the horizontal direction at $y=0.5$](image)

![Figure 3. (a) Non-dimensional radiative heat flux at bottom wall (b) Divergence of radiative flux in the horizontal direction at $y=0.5$](image)
4. Conclusions
The $k$-distribution for mixture of gases has been explored in the current study. Several mixing models have been tested for different scenarios of homogeneous isothermal and non-homogeneous non-isothermal medium. The mixture $k$-distribution obtained from MMM gives promising results compared to other mixing models. However, for higher values of absorption coefficient SMM becomes much more accurate than MMM. HMM gives results in between of SMM and MMM. Error arises from the fact that the mixture $k$-distribution is difficult to obtain from individual gas $k$-distribution.

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