Benchmark Test Cases for Non-Gray Radiative Heat Transfer Calculation using FSK Look-Up Table

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Abstract. Three test cases in the categories of homogeneous non-isothermal, non-homogeneous isothermal and non-homogeneous non-isothermal have been developed to validate the two-dimensional interpolation technique for calculation of non-gray radiative heat flux on the walls of the system. The participating gases H$_2$O and CO$_2$ of different mole fractions and temperatures are considered in different zones of the test cases. HITEMP-2010 database has been used to calculate the absorption coefficients of H$_2$O and CO$_2$ at different mole fractions and temperatures. Further, the random variation of absorption coefficients with spectrum has been reordered in smooth monotonically increasing smooth function using full spectrum k-distribution method (FSK). A look-up table is developed for different mole fractions and temperatures of gases H$_2$O and CO$_2$. The calculation of absorption coefficients at thermodynamic states other than look up table has been performed using two dimensional interpolation techniques. The geometry of test cases have been divided into three zones whose conditions on the first and last zones are same as available in look-up table while interpolation is used for the middle zone. The radiative transfer equation is solved numerically by finite volume discrete ordinate method (FVDOM). The results have been compared with FSK method and have been found that interpolation techniques are giving satisfactory results with extremely less computational resource and time.

1. Introduction

Heat transfer due to radiation plays major role in many engineering applications like combustion, rocket propulsion etc, the radiative heat transfer in participating medium must be accounted. Gray medium is an engineering approximation where radiative properties like absorption and scattering coefficients of medium are constant and spectrum is totally omitted from the context of radiative heat transfer. The accepted fact is that gray approximation does not produce realistic results. The spectral properties of the medium vary drastically with the electromagnetic spectrum. The thermal radiation mostly lies in the visible and infrared regions and participating gases like H$_2$O and CO$_2$ are IR active i.e. they emit and absorb differently at different bands, this makes extremely difficult to do spectral integration for these gases [1], due to these facts and limitations, many researchers have proposed different models which can be classified into line by line (LBL), narrow band models, wide band models and global models. The spectral integration by LBL to those gases is extremely difficult and only performed for bench-marking the solution. Global models are the most promising ones to trade off between computational resource requirement and accuracy. Some of the common global models are spectral line weighted (SLW) [2], absorption distribution function (ADF) [3], full spectrum k-distribution method (FSK) [4],
weighted sum of gray gas model (WSGG) [5]. The absorption coefficient varies abruptly with the electromagnetic spectrum and its calculation is one of the most important part in determining heat transfer by radiation. It is mostly computed from databases like HITRAN-2008, CDS-4000 or HITEMP-2010 [6] for participating gases \( H_2O \) and \( CO_2 \) with low spectral resolution. But performing the radiation calculation on these spectrally varying absorption coefficient is extremely difficult for practical problems. The absorption coefficient of gases can be reordered into monotonically increasing function with respect to non-dimensional Planck function weighted cumulative wavenumber, then an accurate solution of radiative transfer equation can be obtained with few quadrature points unlike to LBL method where computation need to perform hundred million lines. To implement above concept Modest and coworkers [7] suggested to generate k-distributions for various pressures, temperatures, mole-fractions and an efficient scheme for linear interpolation between these tables. In computational domain each cell can be considered as homogeneous and isothermal then FSK can accurately be used for each cell while correlating the absorption coefficient at run-time would not be feasible. In the present work, the linear interpolation technique has been verified in the three canonical test cases of homogeneous non-isothermal, non-homogeneous isothermal and non-homogeneous non-isothermal. The manuscript is organised as methodology in section 2 followed by results and discussions, and finally work is concluded in section 4.

2. Methodology

The accuracy of FSK is comparable to LBL but every time calculation of k-distribution is cumbersome activity. In order to generate database of k-distributions, we need to find absorption coefficients at different temperatures, mole-fractions and pressures, that have been calculated from HITEMP-2010 which contains 11,42,41,164 and 1,11,93,608 transition lines for \( H_2O \) and \( CO_2 \) respectively. The spectral absorption coefficient is calculated from Lorentz profile, and it is a accurate line profile for temperature up to 2000K. In the current study we have considered pressure of 1 bar, eight different temperatures varying between 300 K to 2000K and six different mole-fractions varying from 0 to 1 for both \( CO_2 \) and \( H_2O \). In total we have generated database of around 30 KB size, while the size of spectral absorption coefficients are around 2 GB, which is very large compared to the FSK database. Finally, the reordered absorption coefficient is calculated as below.

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

where index a is taken as 0.3678, number of reordered k points(N) in FSK is 5000, \( k_{\text{min}} \) and \( k_{\text{max}} \) are the minimum and the maximum absorption coefficient available. The skewed distribution is considered to capture lower k-values. The fractional Planck function and non-dimensional cumulative wavenumber g are obtained as

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

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

The above equation represents the spectral variations of absorption coefficient converted into smooth monotonically increasing function. Now, similar accuracy can be obtained with less quadrature points by spectral integration in g domain. These quadrature points can be selected as suggested by Wang and Modest [8].
3. Results and Discussions
Aforementioned methodology for non homogeneous and non isothermal is tested for some of the canonical problems. The details of the test cases are explicated in subsequent sub sections. The radiative transfer equation for all the subsequent test cases are solved numerically by finite volume discrete ordinate method (FVDOM).

3.1. Homogeneous and Non-Isothermal Medium:
Figure 1(a) shows the simple cavity enclosure whose walls are cold and black. The enclosure is trifurcated containing mixture of gases of the same mixture fraction, but different temperatures. The zones on either sides of cavity, FSK lookup table is used while for middle zone k-distribution is interpolated. Figure 1(b) shows comparison result between FSK table and interpolation data sets.

![Figure 1](image1.png)

Figure 1: (a) An enclosure for test case refers to homogeneous and non-isothermal (b) Non-dimensional radiative heat flux on bottom wall

![Figure 2](image2.png)

Figure 2: (a) An enclosure for test case refers to non-homogeneous and isothermal (b) Non-dimensional radiative heat flux at bottom wall
4. Conclusions
The FSK lookup tables have been generated for \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) gases for various mole fractions and temperatures, while interpolation technique is devised for non-homogeneous and non-isothermal medium. These lookup tables and interpolation techniques are tested on three canonical problems and are found to provide acceptable accuracy with drastically reduced computation time. A little difference of results have been observed at higher temperature zone of the enclosure but within 2% of acceptable deviations.

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