NUMERICAL SIMULATION OF RADIATIVE HEAT TRANSFER

by

BABILA RAMAMOORTHY

ROY P. KOOMULLIL, COMMITTEE CHAIR
CHIH-HSIUNG CHENG
PETER M. WALSH

A THESIS

Submitted to the graduate faculty of The University of Alabama at Birmingham,
in partial fulfillment of the requirements for the degree of
Master of Science

BIRMINGHAM, ALABAMA

2008
NUMERICAL SIMULATION OF RADIATIVE HEAT TRANSFER

BABILA RAMAMOORTHY

MASTER OF SCIENCE IN MECHANICAL ENGINEERING

ABSTRACT

Radiative heat transfer is an important physical phenomenon, especially in high speed and high temperature flow applications such as space exploration vehicles. Analysis of aero-thermodynamic environment of re-entry vehicles requires a numerical tool to compute radiative heat transfer, a tool that can be used in coupling with Computational Fluid Dynamics. This thesis presents the development and validation of such computational tools for modeling radiative heat transfer. A generalized grid-based finite volume method is used for solving the radiative heat transfer equation. Solution of the radiative heat transfer equations in the angular domain is carried out in a parallel environment. This numerical approach is validated with different benchmark test cases for gray gas radiation. To enable the simulation of non-gray gas radiation, the full spectrum correlated-\(k\) model is implemented. The results from validation studies, grid sensitivity studies, and parallel performance study are presented in this thesis.
ACKNOWLEDGEMENTS

I wish to express my deepest appreciation and gratitude to my mentor, Dr. Roy Koomullil, and my committee member, Dr. Gary Cheng, for their inspirational guidance, endless support, and abundant patience throughout this work. I also thank Dr. Peter Walsh for serving on my thesis committee and for sharing his valuable knowledge in the field of radiation. I also want to thank Dr. Ramin K. Rahmani for his immense help in this work. Throughout the course of this work, I have greatly benefitted from the knowledge and experience of others. In particular, I would like to acknowledge the help of Dr. Modest’s group at Pennsylvania State University and of Ertan Karaismail at West Virginia University.

I wish to express my appreciation to all of my friends at UAB. A special note of thanks to Lavanya Bhattu, Rohith Kumar, Balapriya Shanmugam, Meenakshi Kushwaha, Balaji S. Venkatachari and Shravan Kumar, who had been a constant source of encouragement and support. A warm thanks to my mother, my family members, and my friend Abhishek for their invaluable support.
TABLE OF CONTENTS

ABSTRACT.................................................................................................................. ii
LIST OF TABLES.............................................................................................................. vi
LIST OF FIGURES......................................................................................................... vii
CHAPTER
1 INTRODUCTION................................................................................................. 1
2 LITERATURE SURVEY............................................................................................ 4
   Overview of Various Models Available to Represent the Spectral Properties of a Medium .................................................................................................................. 4
      Radiative Spectrum .................................................................................................. 5
      Spectral LBL Models ............................................................................................... 6
      Band Models ........................................................................................................... 7
      k-Distribution Models ............................................................................................ 8
      Total Emissivity and Absorptivity Models ............................................................ 9
   Comparison of Various Models to Obtain Radiative Properties .............................. 16
   Overview of Various Numerical Approaches to Predict the Radiative Heat Transfer ........................................................................................................ 18
      Monte Carlo Method ............................................................................................ 18
      Zone Method ......................................................................................................... 19
      Spherical Harmonics Method (SHM) .................................................................... 19
      Discrete Ordinates Method (DOM) ....................................................................... 20
      Finite Volume Method (FVM) ............................................................................... 21
   Comparison of Various Numerical Models for Predicting Radiative Heat Transfer ... 22
3 NUMERICAL APPROACH.................................................................................... 24
   Finite Volume Method ............................................................................................ 24
      Finite Volume Integration ...................................................................................... 26
      Control Volume Treatment .................................................................................. 27
      Spatial Schemes .................................................................................................... 29
      Boundary Condition ............................................................................................. 31
      Treatment for Overhang Problem ......................................................................... 31
      System of Linear Equations ................................................................................. 32
      Improvements to the FVM Solver ......................................................................... 33
   Full Spectrum Correlated-k Model (FSCK) .............................................................. 34
      Implementation of the FSCK model ..................................................................... 35
   Angular Domain Decomposition-Based Parallel Algorithm ................................... 39
<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Comparitive Merits and Demerits of Radiative Spectral Integration Models</td>
</tr>
<tr>
<td>2</td>
<td>Comparitive Merits and Demerits of Radiative Solver Models</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Portions of Spectrum for a Few Absorption Lines where the Fraction of Black Body Energy is Calculated for a Given $C_{abs}$ Value.</td>
<td>13</td>
</tr>
<tr>
<td>2</td>
<td>SLW Spectrum Constructed from the LBL Spectrum.</td>
<td>14</td>
</tr>
<tr>
<td>3</td>
<td>Absorption Coefficient of CO$_2$ at Temperature 1000 K and Pressure 0.1 Bar.</td>
<td>15</td>
</tr>
<tr>
<td>4</td>
<td>Generalized Grid.</td>
<td>26</td>
</tr>
<tr>
<td>5</td>
<td>Ray Defined in Terms of Polar and Azimuthal Angles.</td>
<td>28</td>
</tr>
<tr>
<td>6</td>
<td>Spatial Schemes.</td>
<td>29</td>
</tr>
<tr>
<td>7</td>
<td>Overhang Control Angle in 2D.</td>
<td>32</td>
</tr>
<tr>
<td>8</td>
<td>Schematic of the Parallel Algorithm.</td>
<td>40</td>
</tr>
<tr>
<td>9</td>
<td>Black Square Duct with No Participating Medium.</td>
<td>46</td>
</tr>
<tr>
<td>10</td>
<td>Black Duct with a Participating Medium.</td>
<td>48</td>
</tr>
<tr>
<td>11</td>
<td>3-D Black Duct with a Participating Medium.</td>
<td>50</td>
</tr>
<tr>
<td>12</td>
<td>Radiative Heat Transfer on an Irregular Arc Geometry.</td>
<td>51</td>
</tr>
<tr>
<td>13</td>
<td>Radiative Heat Transfer on a Rhombus.</td>
<td>52</td>
</tr>
<tr>
<td>14</td>
<td>Radiative Heat Transfer on a Cylinder.</td>
<td>54</td>
</tr>
<tr>
<td>15</td>
<td>Radiative Heat Transfer on a Tetrahedral Geometry.</td>
<td>55</td>
</tr>
<tr>
<td>16</td>
<td>Isothermal, Homogeneous Test Case.</td>
<td>58</td>
</tr>
<tr>
<td>17</td>
<td>Non-Isothermal, Homogeneous Test Case.</td>
<td>62</td>
</tr>
<tr>
<td>18</td>
<td>Test Case with Parabolic Temperature Profile.</td>
<td>64</td>
</tr>
<tr>
<td>19</td>
<td>Parallel Performance (Speed up vs. Number of Processors).</td>
<td>65</td>
</tr>
</tbody>
</table>
CHAPTER 1
INTRODUCTION

Radiation is an important mode of heat transfer that has a wide range of applications, from combustion to high speed flows. One of the important applications in which radiation plays a major role is re-entry aero-thermodynamics. For example, in the Apollo mission, it was found that 30% of the total heat transfer rate during re-entry was due to radiation from the shock layer [1]. In re-entry applications, due to the high velocity of the re-entry vehicle, a detached oblique shock is formed in front of the vehicle. This shock layer energizes the gas around the windward blunt surface of the re-entry vehicle and causes very high temperature in this region, resulting in a state of thermo-chemical non-equilibrium in the region behind the shock layer. The high temperature gas produces large radiation because the radiative heat transfer is a function of the fourth power of the temperature. Combinations of large radiative (from high temperature gases) and convective (from high speed flows) heat fluxes contribute to large heat loads on the surfaces of the re-entry vehicle. A Thermal Protection System (TPS) is often employed to protect the surface of re-entry vehicles from such severe aerodynamic heating. An inadequate or wrong choice of TPS material might result in the failure of the TPS, whereas excess or dense insulation results in the addition of unnecessary weight to the vehicle. An appropriate margin has to be determined for the thickness of the thermal insulation in order to arrive at the proper amount of TPS material to be added to the structure. This necessitates a reliable, accurate prediction of the radiative and convective heat transfer to design the
TPS of a re-entry vehicle. The experimental study of the application, using either ground or flight tests of this type is very expensive, complicated, and subject to large uncertainties. Numerical simulation of radiation is a convenient, low-cost approach to calculate the radiative heat loads associated with such a scenario. Thus the numerical heat transfer provides a viable option in spite of its sensitivity to physical, chemical, and numerical model parameters. A detailed report on the numerical simulation of aero-thermodynamics around the re-entry vehicle and the uncertainty associated with such a study has been reported in the literature [2-4]. An assessment of numerical modeling of non-equilibrium radiative heat transfer has been presented by Sharma et al [5].

Electromagnetic radiation is continuously emitted from all substances [6]. Thermal radiation forms an important part of electromagnetic radiation due to its practical significance. The wavelength of interest in the thermal radiation spectrum includes the long-wave portion of the ultraviolet spectrum, the visible light region and the portion of the infrared spectrum up to a wavelength of 1000 μm. Thermal radiation, unlike conduction and convection, depends on the temperature difference raised to its fourth power. Hence, at high temperatures, radiation becomes more important than conduction and convection. Another important property of radiation is that, unlike conduction and convection, it does not require an intervening medium to travel.

The most important property that complicates the numerical computation is the spectral and directional dependence of radiation. They are also a function of the temperature, pressure, and composition of the gas mixture. Numerical computation methodologies have to account for all these properties while computing radiative heat transfer properties. This thesis addresses such issues in computing radiative heat transfer.
The objectives of this thesis are

i. to develop a numerical tool that can be used in combination with computational fluid dynamics (CFD) solvers to predict the radiative heating in high speed re-entry problems,

ii. to investigate numerical approaches for evaluating the radiation intensity to compute the radiative heat transfer, and

iii. to explore numerical models for estimating the radiative properties of a gray-gas medium. This thesis also presents the validation of the developed tools with benchmark test cases.

Chapter 1 is the introduction. There exists a wide variety of methods to model the spectral properties of the medium and to compute radiative heat transfer. A survey of the literature and a comparative study of these existing models are given in Chapter 2. The numerical approach that is being used in this study for the solution of the radiative heat transfer equation is presented in Chapter 3. Chapter 4 presents the results and discussion from the validation studies, followed by conclusions and suggestions regarding possible future work in Chapter 5.
CHAPTER 2
LITERATURE SURVEY

Like any other physical phenomena, radiative heat transfer can be studied using experimental, theoretical or numerical approaches. The experimental study of radiative heat transfer in actual flight test conditions can be very expensive and impractical. The analytical approach is restricted to simplified cases only, since arriving at an analytical solution for realistic cases is an extremely difficult and sometimes impossible task. Numerical modeling thus serves as the most effective choice for the study of radiative heat transfer.

Numerical simulation of radiative heat transfer involves two steps. The first step involves the evaluation of radiative properties by analyzing the spectrum of the participating medium for a set of given conditions, such as temperature, pressure, mole fraction, and particulates. The second step is to compute the radiative heat transfer using the estimated radiative properties from the first step. This section details the various models available to obtain spectral radiative properties as well as different numerical approaches to compute the radiative heat transfer.

Overview of Various Models Available to Represent the Spectral Properties of a Medium

Due to the spectral dependence of radiative properties, the numerical analysis of radiation requires integration over the spectrum. This requires the knowledge of the spectrum of the participating species, which is also dependent on temperature, pressure, and
the composition of the gas mixture. There are several approaches available in the literature to obtain these properties with different levels of accuracy. Some of the most popular methods are detailed in this literature survey.

Equilibrium radiative heat transfer is important and has a wide range of applications, but the radiation of high temperature gases involves non-equilibrium conditions and necessitates the study of non-equilibrium radiation. Thermal or chemical non-equilibrium results in the change of the spectral properties of the gas, since radiative properties such as absorption coefficient, and emissivity are functions of temperature, partial pressure, species concentration, etc. Any change in these parameters results in a change in the spectrum of the gas [7] and thus the resulting radiative heat transfer, so the study of non-equilibrium gas radiation requires the integration of the radiative transfer equation over the spectral frequency or wavelength. The purpose of this section is to give a brief note on the different approaches available to carry out the spectral integration and to discuss their relative merits and demerits.

Radiative Spectrum

The atoms and molecules of a radiating species populate certain discrete sets of energy levels depending on local conditions, such as temperature, pressure, etc. These atoms or molecules change to higher or lower energy levels from their original state by absorbing or emitting photons. Such emission or absorption of a photon by a molecule results in the discrete change of rotational and vibrational energy levels in molecules or in the change of electron orbits. It should be noted that the emitted or absorbed photon should have the appropriate frequency to change the energy state to higher (absorption)
or lower (emission) discrete energy levels. This change results in a spectral line in an otherwise continuous spectrum [8]. These spectral lines are thin lines that occur over a tiny but finite range of wave numbers. Ideally, the spectral lines should be very thin, but they are broadened due to such reasons as collision broadening, natural line broadening (by Heisenberg’s uncertainty principle), and Doppler broadening. More discussions on spectral lines and line broadening can be found in the literature [6, 8]. Since thermal radiation is due to the energy propagated by these photons, it is important to analyze the spectrum of a species when computing the radiative heat transfer.

The models used for defining the radiative properties of high temperature gases are broadly classified in three types, depending on how they treat the spectrum [7]:

i. Spectral Line By Line Models (LBL)

ii. Band Models

iii. Global Models (total emissivity and absorptivity models)

*Spectral LBL Models*

The LBL models [8] are the most accurate but computationally the most expensive models. In this model, the variation in spectral properties is accounted for by calculating the spectral properties over the detailed molecular spectrum of gases, for all the spectral lines. Considering the fact that radiating species have millions of spectral lines, the accuracy achieved by the LBL models is outweighed by their computational expense. These models are unrealistic for large practical applications with current computer power and are mainly used in validating other numerical approaches. One such study where the LBL model has been used to generate benchmark results has been done by Riviere et al [9]. There have also been some efforts to alleviate the computational cost of the LBL me-
methods by modifying the algorithms for calculating absorption coefficients without compromising the numerical accuracy [10].

**Band Models**

The band models [11,12] are based on averaging radiative properties over a spectral band. Band models compute average emissivity and absorptivity over either a narrow or a wide band by assuming a profile for spectral lines within the band. Band models are divided into two types, Narrow Band Model (NBM) and Wide Band Model (WBM), based on the width of the band used in averaging.

*Narrow Band Model*

NBM compute the spectral properties within a narrow band by assuming a profile for line shapes, width, and spacing within a narrow spectral interval. The two most popular line arrangements for NBM are

i. uniformly spaced lines with equal intensities (Elsasser or Regular Model [11]).

ii. random exponential line intensity distribution and random line positioning based on uniform probability distribution (Goody or Statistical Model [11]).

Although NBM and LBL models are the most accurate models to compute the radiative properties of gas mixtures, they are computationally expensive for practical applications. NBM, like LBL models, are also used to generate benchmark results for validating other models.
**Wide Band Model**

WBM are computationally less expensive than the NBM because averaging over a wider band width is employed to compute the spectral properties. Many simplified WBM have been proposed. A simplified WBM that computes the cumulative-$k$ (absorption coefficient) distribution function has been developed by Marin *et al* [13]. The Exponential Wide Band Model (EWBM) is a popular WBM and was based on the idea that the absorption of gases is largely confined to a few vibrational-rotational bands in the infrared region. In addition, EWBM does not require excessive computational power like narrow band or LBL models, since it uses simple expressions to evolve the radiative properties. These models do not rely excessively on databases since they are based on general expressions that are mostly applicable to combustion problems. The main limitation of EWBM is in treating surface-surface radiation problems, since they cannot handle wall interactions efficiently.

**k-Distribution Models**

The $k$-Distribution models differ from band models in that they replace the spectral integration by integration over the absorption coefficient, $k$. The absorption coefficient is reordered within a band by using a cumulative $k$-distribution function, $\bar{g}_i(k) = \int_0^k f_i(k).dk$, where $f_i(k)$, is interpreted as the fraction of the absorption coefficient lying in the interval between $k$ and $k+dk$ in the spectral region for $i^{th}$ band of the gas. Physically, $\bar{g}_i(k)$ is the fraction of the absorption coefficient that has a value less than $k$, within the spectral frequency interval, $\Delta \nu_i$. Correlations are developed to compute the cumulative distribution functions for different gases at different temperatures and pressures. Un-
like the NBM and EWBM, $k$-distribution models have the limitation that new correlations must be computed whenever the temperature or total pressure of the gas is changed.

**Total Emissivity and Absorptivity Models**

The radiative transfer equation (RTE) can be written in the most basic form in terms of the absorption coefficient. The band models and the $k$-distribution methods compute either emissivity, absorptivity, or transmissivity as output. Therefore, to couple these models with an arbitrary RTE solver, either

i. the RTE needs to be rewritten in terms of transmissivity or other radiative properties, or

ii. the absorption coefficient has to be computed from the measured radiative properties.

There is also a need to specify an associated pathlength when transmissivity or other properties are computed as output. Though literature does exist, regarding the use of band models, rewriting the RTE in terms of transmissivity [11], this approach has been tested only on problems of simple geometries.

To overcome these problems, several total emissivity and absorptivity models have evolved that can compute the absorption coefficient as output. These models can be used with arbitrary RTE solvers. In addition, global or total emissivity models avoid the need to do a spectral integration of the RTE solver, thus saving required computation time. These models are relatively simple to formulate and have been successfully applied over a wide range of temperatures and pressures. They offer a very attractive choice, es-
pecially for large practical problems. Some of the most commonly used global models are discussed in this section.

**Weighted Sum of Gray Gases Model (WSGG)**

The WSGG model [14] is one of the most widely used global models. This model involves formulating mathematical expressions that are evolved based on an existing total emissivity database for a set of reference conditions. These expressions are then used to compute the total radiative properties of gases at different conditions [15]. The idea behind the WSGG model, and for that matter, most global models, is to represent a non-gray gas property by using a weighted sum of a few fictitious gray gas properties.

The total emissivity of the WSGG model is evaluated from the following expression [15]:

$$
\varepsilon = \sum_{i=0}^{l} a_{\varepsilon,i}(T)[1 - e^{-k_i p S}]
$$

(2.1)

where $a_{\varepsilon,i}$ denotes the emissivity weighting factors for the $i^{th}$ gray gas, and the temperature dependency is accounted for through $a_{\varepsilon,i}$. $k_i$ is a curve fitting constant. Both these coefficients can be interpreted in two ways: either the coefficients are evaluated mathematically from curve fitting, or $a_{\varepsilon,i}$ can be interpreted physically as a fractional amount of the black body energy in the spectral region where the gray gas absorption coefficient, $k_i$ exists.

$p$ denotes partial pressure and $S$ denotes path length. The absorption coefficient for $i = 0$ represents the regions where the spectral absorption lines are absent (spectral windows) and where transmittance is 1.0.

The weighing factor for $i = 0$ is evaluated as [15]

$$
a_{\varepsilon,0} = 1 - \sum_{i=1}^{l} a_{\varepsilon,i}
$$

(2.2)
The temperature dependency of the weighing factors can be given by the polynomial of the order of $J-1$ as \[15\]
\[
a_{\epsilon,i} = \sum_{j=1}^{l} b_{\epsilon,i} T^{j-1}
\]
(2.3)
where $b_{\epsilon,i}$ is the emissivity gas temperature polynomial coefficients, $J$ is the desired order of accuracy for the polynomial fit, and $l$ is the number of fictitious gray gases. The absorption and polynomial coefficients are evaluated by fitting equation 2.3 to a table of total emissivities.

A similar expression has been evaluated for total absorptivity, but taking into account the irradiation temperature of the surfaces ($T_\gamma$) surrounding the gas. The absorptivity is given by \[15\]
\[
\alpha = \sum_{i=0}^{l} a_{\alpha,i}(T, T_\gamma) \left[ 1 - e^{-k_i \rho_s} \right]
\]
(2.4)
where $a_{\alpha,i}$ is the absorptivity weighing factor represented by the $K$ order polynomial as, \[15\]
\[
a_{\alpha,i} = \sum_{j=1}^{l} \left[ \sum_{k=1}^{K} c_{\alpha,i,j,k} T_\gamma^{k-1} \right] T^{j-1}
\]
(2.5)
where $c_{\alpha,i,j,k}$ are the absorptivity polynomial coefficients.

The absorption and polynomial coefficients are obtained by using curve fitting to the pre-tabulated values of total emissivity and absorptivity. These tabulated values are obtained by using either LBL models or band models \[15\]. An extended WSGG model to account for the presence of particulates in a non-gray gas has been presented by Yu et al \[16\].
Spectral Line-Based Weighted Sum of Gray Gases Model (SLW)

The Spectral Line-Based WSGG models [17,18] are generated directly from the LBL spectra of a given gas, unlike WSGG models, which are based on curve fitting to the total emissivity data. The SLW model can be used with arbitrary RTE solvers, since it outputs the absorption coefficient.

As in the WSGG model, in the SLW model, a non-gray gas is represented by a mixture of gray gases with weights associated to each gray gas. The absorption coefficient and weights associated with each gray gas is determined as follows:

**Determination of absorption coefficients for each gray gas.** As a first step to calculate the absorption coefficients for a gray gas, an absorption cross section vs. wave number plot is generated from the spectral database. A histogram representation of this plot is generated with a small number of absorption cross sections \( (C_{\text{abs}}) \). Suppose there are \( j = 1 \) to \( J \) number of absorption cross sections, then the \( j^{th} \) gray gas absorption coefficient is defined as

\[
k_j = N \times C_{\text{abs},j}
\]

where \( N \) is the molar density of the gas evaluated from the equation of state.

**Determination of gray gas weights.** The histogram representation calculated from the previous step is used to calculate an absorption line black body distribution function (ALBDF), as shown in equation 2.6. The ALBDF is evaluated for each gray gas \( j \), using the following expression [17]

\[
F_s(C_{\text{abs}},T_b,T_g,P_{\text{Tot}},Y_j) = \frac{1}{\sigma T_b^4} \sum_i \int_{\Delta \eta} \int_{\eta_{(C_{\text{abs}},T_b,P_{\text{Tot}},Y_j)}} E_{\eta}(\eta,T_b) d\eta
\]  

(2.6)
where $\sigma$ is Stephan-Boltzmann Constant

$E_{\eta}$ is Planck’s function evaluated at wave number $\eta$

$T_b$ is the black body source temperature

$T_g$ is the gas temperature

$P_{Tot}$ is the total pressure

$Y_j$ is the mole fraction of the broadening species

‘$i$’ refers to $i^{th}$ spectral segment and summation is performed over the entire spectrum. This ALBDF can be physically defined as the fraction of the total black body energy contained in the regions where $C_{abs,\eta}$ is lower than a given value, $C_{abs}$.

A sample plot of fraction of the black body energy, between absorption cross section values $\tilde{C}_{abs,j}$ and $\tilde{C}_{abs,j+1}$ is shown in Fig 1. The weight factor associated with a gray gas $j$, based on the black body energy associated with $j$, is given by [17]

$$a_j = F_s(\tilde{C}_{abs,j+1}, T_b, T_g, P_{Tot}, Y_j) - F_s(\tilde{C}_{abs,j}, T_b, T_g, P_{Tot}, Y_j)$$

Figure 1. Portions of Spectrum for a Few Absorption Lines where the Fraction of Black Body Energy is Calculated for a Given $C_{abs}$ Value.
A sample of the SLW spectrum constructed from the LBL spectrum through histogram representation is shown in Fig 2. Each $C_{abs}$ shown in Fig 2 is represented using a gray gas, $j$. As in the WSGG model, the RTE for a gray gas is solved for all the gray gases, and the total radiative intensity is the sum of intensities due to all of the gray gases.

![Figure 2. SLW Spectrum Constructed from the LBL Spectrum.](image)

**Full Spectrum Correlated-k Model (FSCK)**

The Full Spectrum Correlated-k (FSCK) model is based on re-ordering the $k$-distribution for the full spectrum [19]. The correlated-$k$ model is based on the fact that inside a small spectral interval, the precise position of the spectral line (i.e. $\eta$ or wave number, $\lambda$) is not important. The FSCK model extends this idea to the full spectrum. To illustrate this fact further, consider the RTE for a given spectral wavenumber, $\eta$ [19].

$$\frac{dl_{\eta}}{ds} = \kappa_{\eta}(l_{b\eta} - l_{\eta}) + \frac{\sigma_{\eta}}{4\pi} \int l_{\eta}(s')\phi(s', s)d\Omega' \quad (2.8)$$
It can be seen from equation 2.8 that the radiative intensity (along a path $s$) at a given wavenumber, $I_\eta$, depends on such properties as the Planck function, $I_{b\eta}$, the scattering phase function, $\phi(s', s)$, and the raw absorption and scattering coefficients, $\kappa_\eta$ and $\sigma_{s\eta}$. $\Omega'$ is the integration variable for the angular direction. In this equation, $I_{b\eta}$ is the only variable that is a direct function of $\eta$. If a sufficiently narrow spectral interval is considered for spectral integration (in which $I_{b\eta}$ can be assumed constant), it is clear that $I_\eta$ depends only on $\kappa_\eta$ and $\sigma_{s\eta}$. If the medium is assumed to be non-scattering for simplicity, then $I_\eta$ depends only on $\kappa_\eta$. Even in such a narrow spectral interval, $\kappa_\eta$ has a chaotic variation and attains the same value many times, and the same $I_\eta$ value is also attained many times.

This is evident from the $\kappa_\eta$ vs $\eta$ plot shown in Fig 3 for the CO$_2$ spectrum over a small wavenumber interval of 10 cm$^{-1}$ at a temperature of 1000 K and a pressure of 0.1 bar.

Figure 3. Absorption Coefficient of CO$_2$ at Temperature 1000 K and Pressure 0.1 Bar.
To avoid repeating the calculations where $I_\eta$ attains the same value, the spectral absorption coefficient can be re-ordered into a monotonically increasing function, and the repeated calculations can be avoided.

Re-ordering of the spectral absorption coefficient. If the medium is homogeneous or the absorption coefficient obeys the so-called scaling approximation [19], then

$$\kappa = k(\eta)u(T, p, \chi)$$

(2.9)

where $u$ is the scaling function.

$T$, $p$, and $x$ are the local state variables namely temperature, pressure and species mole fraction.

$k(\eta)$ can be re-ordered in terms of an equivalent Planck function $g$, i.e., $k(\eta)$ vs $\eta$ can be replaced by $k(g)$ vs $g$, where $k(g)$ is a monotonically increasing function. The RTE can also be rewritten in terms of $k(g)$ and solved for a few quadrature points in the $k(g)$ vs $g$ function. The resultant intensity is obtained by the weighted sum over $I(g)$ of all the quadrature points. More details of this model can be found in the next section.

The FSCK model is claimed to be very accurate within the limitations of a global model (gray walls, gray scattering) and scaling approximation. In addition, it has been shown that the WSGG model is simply an approximation of the FSCK model proposed by Modest [19].

Comparison of Various Models to Obtain Radiative Properties

From this discussion of the various models, it can be seen that the LBL methods and NBM are the most accurate models to represent the radiative properties of a medium, but they are computationally very expensive. Though the WBM are computationally
cheap, they pose a problem when incorporated into the RTE solvers since they output properties like transmissivity, whereas RTE solvers are based on an absorption coefficient. The WBM also requires the specification of a path length, which becomes difficult to define in the case of complex geometries. The global models serve as the best alternative, since they are computationally cheap and can be easily integrated with arbitrary RTE solvers. A comparative list of the merits and demerits of these models is shown in Table 1.

Table 1. Comparative Merits and Demerits of Radiative Spectral Integration Models.

<table>
<thead>
<tr>
<th>Models</th>
<th>Accuracy</th>
<th>Computational Expense</th>
<th>Integration with RTE Solver</th>
</tr>
</thead>
<tbody>
<tr>
<td>LBL Models</td>
<td>Very Accurate</td>
<td>Highly Expensive</td>
<td>Directly Integrable</td>
</tr>
<tr>
<td>NBM</td>
<td>Very Accurate</td>
<td>Highly Expensive</td>
<td>Not Directly Integrable</td>
</tr>
<tr>
<td>WBM</td>
<td>Less Accurate</td>
<td>Less Expensive</td>
<td>Not Directly Integrable</td>
</tr>
<tr>
<td>Global Models</td>
<td>Less Accurate</td>
<td>Least</td>
<td>Directly Integrable</td>
</tr>
</tbody>
</table>

The spectral line-based weighted sum of gray gases model is a good choice of global models since it is based on the direct approximation of the LBL absorption spectrum and is computationally cheaper compared to the LBL and NBM methods. The SLW model has also been found to perform better than the wide band correlated-\(k\) model [20] and can also handle inhomogeneous gas mixtures efficiently [21]. The FSCK model proposed by Modest is thought to be a more efficient numerical approach [19]. It has been shown by Modest that “the WSGG model is only a crude approximation of the FSCK model” [19]. It is also claimed that the FSCK model is more accurate than the WSGG and SLW models and can handle inhomogeneous and non-isothermal applications. For these reasons, the FSCK model was implemented and assessed in this thesis research.
Overview of Various Numerical Approaches to Predict the Radiative Heat Transfer

There are several numerical approaches available to solve for the radiation heat transfer [8]. The ones used most extensively are the Zone Method, Monte Carlo Method, Spherical Harmonics Method, Discrete Ordinates Method (DOM), and Finite Volume Method (FVM). These methods and their relative merits and demerits are summarized in this section.

Monte Carlo Method

The Monte Carlo method [22] is a numerical method based on an indeterministic statistical approach. This approach is particularly helpful in radiation, since the deterministic approach is complicated by the combined spectral and spatial dependence of the radiative transfer. In addition, the solution of RTE requires both spatial and angular integration, other than spectral integration. Hence the Monte Carlo solutions are less complicated to compute as compared to deterministic approach, and there is no approximation involved in the solution process. The Monte Carlo algorithm can easily be parallelized into embarrassingly parallel computations, which is a big advantage in terms of large problems. Because of these distinct advantages, a large number of radiation problems have been solved using Monte Carlo techniques. A thorough review of Monte Carlo techniques for solving radiative heat transfer has been presented by Howell [22].

The drawback of the Monte Carlo method is the large computational times involved. Since this method is based on statistical characteristics, the larger the number of samples evaluated, which requires larger computational resources, the higher the accura-
cy. Because of this, the trade-off between accuracy and computational time is critical in this method.

Zone Method

The main idea of the zone method [23] is to compute exchange areas of participating volumes and surfaces. The enclosure surfaces are divided into smaller areas, and the participating media volumes are divided into smaller volumes. The radiation exchange between the areas and volumes are computed based on their exchange areas. The direct exchange areas are areas between two surfaces that are directly involved in energy transfer, and total exchange areas are surfaces that eventually exchange radiative energy among them. The zone method is considered a powerful approach for computing radiative heat transfer, but evaluation of the direct exchange areas requires the calculation of integrals up to six dimensions, thus requiring large computational resources. This restricts the applicability of the zone method to practical engineering problems. The computational resource issue has been addressed by reducing the dimensions of integrals for the direct exchange area calculation as presented in the literature [24]. Another disadvantage with the zone method is the difficulty in coupling with CFD codes.

Spherical Harmonics Method (SHM)

The SHM [8] is based on obtaining an approximate solution of an arbitrarily higher order by transforming the equation of radiative transfer into a set of partial differential equations. The great advantage of this method is that the set of transformed partial differential equations is simpler than the original RTE. The drawback of this method is
that low-order approximations are usually accurate only in optically thick media, and accuracy improves slowly for higher order approximations. The mathematical complexity increases as the accuracy improves.

**Discrete Ordinates Method (DOM)**

The DOM [25,26] is a popular numerical method to handle radiation problems. In this method, the computational domain is discretized in both spatial and angular domains to account for the spatial and directional variation of the radiation intensity. The angular integration to obtain the total intensity is done by using numerical quadrature over all of the angles. In an $S_n$ discrete ordinates method, numerical solutions are found by solving the RTE for a set of $n \times (n+2)$ discrete directions, discretizing the solid angle of $4\pi$ followed by numerical quadrature. The spatial discretization procedure is same as the finite volume method. This method is computationally cheaper compared to the zone, Monte Carlo, or SHM methods. This method can also be easily coupled with CFD solvers because of the common control volume approach. Though the DOM is computationally efficient, it is not very accurate for all kinds of radiative heat transfer problems. For example, DOM does not offer flexibility in angular discretization. This allows the radiative intensity variation to be accounted for in only a few predetermined directions. This leads to inaccuracies in the numerical solution called ray effects. If there is a radiative source present in the computational domain, depending on whether or not a predetermined direction falls on the same angle, the source may or may not be resolved properly. If the medium is scattering, then the ray effect is less acute, since scattering allows information exchange between different directions, but this problem is acute in a non-scattering me-
dium. Apart from angular discretization, the DOM also has problems of numerical smearing and dispersion. Some approaches have been employed to address this problem by using bounded, high-resolution differencing schemes [25]. Another drawback is that DOM is not in conservation form and does not ensure the conservation of radiation energy.

In a study by Fiveland [26], the $S_4$ and $S_6$ DOM solutions seem to compare well with the zone method solutions for radiation in black or gray rectangular enclosures. In a black square enclosure with absorbing medium, the DOM solutions are shown to be more accurate than a higher order SHM approximation.

*Finite Volume Method (FVM)*

Similar to the DOM, the FVM [27-32] discretizes the computational domain in both spatial and angular directions to account for the spatial and directional variations of the radiation intensity. For spatial discretization, the solution domain is discretized by a computational mesh that defines a set of nodes and control volumes. The FVM differs from DOM only in the angular discretization procedure. For angular discretization, the angular space $4\pi$ at any spatial location is discretized into discrete, non-overlapping solid angles $\omega_i$. This is done in 3-D space for each problem by specifying the number of polar and azimuthal angles. Like CFD, the FVM is also based on the conservation principle. The radiant energy is conserved within a control angle, a control volume, and also within the solution domain. The main advantage of the FVM, is that it offers the user the flexibility to choose any kind of spatial and angular discretization that best captures the physics of the given problem. The FVM is also computationally cheaper and comparable to the DOM method in terms of computational resources. It can also be coupled with CFD.
codes easily, as both can share the common control volume approach. The boundary
treatment in the FVM is also similar to that in CFD. A detailed description of the FVM
methodology is discussed in chapter 3.

Comparison of Various Numerical Models for Predicting Radiative Heat Transfer

The previous sections briefly explained various numerical methods available to solve radiative heat transfer problems. Although the Monte Carlo and zone methods are the most accurate methods available, they require large computational resources for practical applications. The DOM and FVM are more practically realistic methods for engineering problems, with the FVM offering a more flexible angular discretization than the DOM method. A comparative assessment of these two methods has been reported by Kim and Huh [30], and a study comparing the zone method, DOM, and FVM is reported by Coelho [33]. The relative merits and demerits of all of these methods have been presented in Table 2.

Table 2. Comparative Merits and Demerits of Radiative Solver Models.

<table>
<thead>
<tr>
<th>Models</th>
<th>Accuracy</th>
<th>Computational Complexity/Expense</th>
<th>Integration with CFD Solvers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monte Carlo Zone Method</td>
<td>Highly Accurate Highly Accurate</td>
<td>Less complex; very expensive  More complex; more expensive</td>
<td>Not readily integrable</td>
</tr>
<tr>
<td>Spherical Harmonics Method</td>
<td>Good Accuracy</td>
<td>More complex; not so expensive</td>
<td>Not readily integrable</td>
</tr>
<tr>
<td>Discrete Ordinates Method</td>
<td>Good Accuracy</td>
<td>Less complex; less expensive</td>
<td>Readily integrable</td>
</tr>
<tr>
<td>Finite Volume Method</td>
<td>Good Accuracy</td>
<td>Less complex; less expensive</td>
<td>Readily integrable</td>
</tr>
</tbody>
</table>

The FVM approach has been successfully demonstrated for structured, unstructured, and non-orthogonal meshes. FVM is an ideal candidate for solving the RTE, espe-
cially when coupled with CFD methods and at less computational expense. For these reasons, the current study uses the FVM method for the solution of the RTE.
CHAPTER 3

NUMERICAL APPROACH

In the numerical approach for calculating radiative heat transfer, the RTE must be integrated in the spectral, spatial, and angular domains. As discussed in Chapter 1, FVM has been used to perform spatial and angular integration, and the FSCK method has been used to perform the spectral integration. This chapter discusses

i. the implementation of FVM and FSCK methods

ii. the parallel algorithm implementation based on angular domain decomposition

Finite Volume Method

In this study, a generalized grid-based FVM has been used [7,34] to perform spatial and angular integration of the RTE. The governing equation for radiative heat transfer (RTE) in a gray absorbing, emitting, and scattering medium along a direction $s$ can be written as [7].

$$\frac{dI(\hat{r}, \hat{s})}{ds} = -\left[k(\hat{r}) + \sigma_s(\hat{r})\right]I(\hat{r}, \hat{s}) + S(\hat{r}, \hat{s})$$  \hspace{1cm} (3.1)

where

$I$ is the intensity of radiation

$k$ is the absorption coefficient

$\hat{r}$ is the position vector

$\hat{s}$ is the direction vector

$\sigma_s$ is the scattering coefficient
$S$ is the source term

The first term on the right-hand side of equation (3.1) is the attenuation of radiative intensity through absorption and out-scattering. When a beam of radiation travels along a path ($\hat{s}$), some amount of the radiation is absorbed by the medium in which it is travelling. The amount of radiation absorbed depends on the medium in which it is travelling and the local temperature, pressure, species composition and concentration. These factors are accounted for by the absorption coefficient, $k$ and the attenuation due to this absorption is given by $kI$. Similarly, the loss of radiative intensity due to scattering of the radiative intensity from the direction, $\hat{s}$ to other directions (out-scattering) is given by $\sigma_s I$.

The second term in the right-hand side of equation (3.1) is the source term given by

$$S(\hat{r}, \hat{s}) = k(\hat{r})I_b(\hat{r}) + \frac{\sigma_s(\hat{r})}{4\pi} \int_{4\pi} l(\hat{r}, \hat{s}') \Phi(\hat{s}', \hat{s}) d\omega'$$

where

$I_b$ is the black body intensity

$l(\hat{r}, \hat{s}')$ is the intensity at $r$ within the solid angle $d\omega'$ in the direction $\hat{s}'$

$\Phi(\hat{s}', \hat{s})$ is the scattering phase function from direction $\hat{s}'$ to direction $\hat{s}$

$\omega'$ is the integration variable for angular integration

The source term represents the augmentation of the radiation intensity due to emission and in-scattering. The medium presented along the path of radiation will emit radiation according to the local state variables, which increases the radiative intensity and is given by $kI_b$. There is also an increase in intensity due to the scattering from other di-
rections into the radiation path (§). This is termed as in-scattering and is calculated as shown in the second term in the right-hand side of the source term equation (3.2).

*Finite Volume Integration*

The main difference between other modes of heat transfer (convection and conduction) and radiation is that the radiative heat transfer occurs simultaneously in all directions from a point. Hence to compute radiative heat transfer, the RTE needs to be integrated in spatial and angular directions. To achieve the spatial and angular (directional) integration of the RTE, the FVM discretizes the spatial domain into discrete control volumes (cells) and discretizes the angular domain into discrete control angles. The FVM solver used in this study is a generalized grid based FVM which can handle arbitrary control volumes and control angles. A typical arrangement of control volumes on a generalized grid and a control angle are shown in Fig 4.

![Diagram of Control Volumes and Control Angle](image)

(a) Control Volumes  
(b) Control Angle

Figure 4. Generalized Grid.
In every (control volume) cell, there is an intensity associated with each control angle. The RTE is integrated over the control volume for a given direction defined by the control angle. To perform this integration, the radiative heat transfer to the surfaces of the control volume at a given direction is approximated by an algebraic correlation involving the geometry and cell average values. This correlation is detailed in the next section.

If scattering is absent, the intensities in different directions can be decoupled and can be solved independently for each direction. This process can be repeated for all directions. The resultant intensity in a control volume is calculated by adding the intensities from all directions [7].

**Control Volume Treatment**

The discretization of the RTE defined in Equation (3.1) along an arbitrary direction \( i \) (Fig 5) and a control angle, \( \omega_i \), will result in the following algebraic equation [35]:

\[
\sum_f J_f i_{if} = [-(k + \sigma_s)I_{i0} + S_i]\omega_i \Delta V_0
\]

where

- \( I_{if} \) is the intensity associated with the direction \( i \) at the face \( f \) of the control volume,
- \( I_{i0} \) is the intensity at the centre of the control volume in the direction \( i \)
- \( \Delta V_0 \) is the volume of the cell

The geometric parameters appearing in equation (3.3) can be defined as follows. Let a ray passing along the direction \( i \) be denoted as \( \hat{s} \), as shown in Fig 5. In this Fig., \( \theta_i \) and \( \phi_i \) are the polar and azimuthal angles subtended by the centroid of the solid control angle. This ray is defined in the 3-D space in terms of the cylindrical co-ordinates and is represented mathematically as [35]
The control angle corresponding to this direction is \( \omega_i \) and is given by [35]

\[
\omega_i = \int_{\Delta \varphi} \int_{\Delta \theta} \sin \theta \, d\theta \, d\varphi = 2 \sin \theta_i \sin \left( \frac{\Delta \theta}{2} \right) \Delta \varphi
\]

(3.5)

This integration is exact [35], i.e.,

\[
\sum_i \omega_i = 4\pi
\]

(3.6)

The geometric factor, \( J_f \) is defined as [35]

\[
J_f I_{lf} = I_{lf} \mathbf{A} \cdot \int_{\Delta \theta} \int_{\Delta \varphi} \hat{s} \sin \theta \, d\theta \, d\varphi
\]

(3.7)

Figure 5. Ray Defined in Terms of Polar and Azimuthal Angles.

Equation (3) can be simplified as [35]

\[
J_f I_{lf} = I_{lf} \mathbf{A} \cdot \hat{S}_i
\]

(3.8)

where

\( \mathbf{A} \) is the surface area of the faces of the control volume and

\[
\hat{S}_i = \sin \varphi_i \sin (0.5\Delta \varphi) (\Delta \theta - \cos 2\theta_i \sin \Delta \theta) \hat{i} + \cos \varphi_i \sin (0.5\Delta \varphi) (\Delta \theta - \cos 2\theta_i \sin \Delta \theta) \hat{j} + 0.5\Delta \varphi \sin 2\theta_i \sin \Delta \theta \hat{k}
\]

(3.9)
In these equations, the unknowns are the radiative intensity at a given direction \( i \) at the cell centre and the cell faces, i.e., \( I, I_{if} \), respectively. There are two unknowns and only one equation (RTE). To close this system of equations, the radiative intensity at the cell face, \( I_{if} \) must be expressed in terms of a cell centre value, \( (I) \), by using one of the following spatial schemes in the RTE solver.

**Spatial Schemes**

Two different spatial schemes are available in this solver, the step and exponential schemes.

![Spatial Schemes](image)

**Figure 6. Spatial Schemes.**

*The Step Scheme.* The step scheme is similar to the first-order upwind scheme in CFD. In this scheme [36], the intensity at the face for a given direction \( s \), \( I_{if} \) can be calculated in terms of the intensity at the upstream cell value, \( I_{i,u} \), by [7]

\[
I_{if} = I_{i,u}
\]  

(3.10)

Here \( I_{i,u} \) is the value of \( I_i \) in the upwind cell. In Fig 6, upwind cells for different faces of cell P are shown schematically for the direction indicated in the figure.
The Exponential Scheme. The exponential spatial differencing scheme [27,36] is a higher order spatial scheme that takes into account the exponential decay of the radiative intensity along the optical path in the cell. Considering the path shown in Fig 6, the intensity at the face, $I_f$, can be calculated in terms of the intensity at the upstream face, $I_u$, by [27]

$$I_f = I_u e^{-(\beta_m)\rho d_u} + \left( \frac{s_m}{\beta_m} \right) \left( 1 - e^{-(\beta_m)\rho d_u} \right) \quad (3.11)$$

where

$\beta_m, s_m$ are the modified extinction coefficient and modified source term, respectively, which are given as

$$\beta_m = \beta - \frac{\sigma_s}{4\pi} \phi^{l'l} \Delta \Omega' \quad (3.12)$$

and

$$s_m = \kappa I_b + \frac{\sigma_s}{4\pi} \sum_{l' \neq l, I = 1 \ldots M} I^{l'} \phi^{l'l} \Delta \Omega' \quad (3.13)$$

where

$\phi^{l'l}$ is the average scattering phase function from a control angle $l'$ to a control angle $l$ and

$$\beta = (k + \sigma_s) \quad (3.14)$$

This exponential scheme is implemented in two ways in the current RTE solver. In the first approach, the distance $d_u$ is calculated as the length of the ray segment that extends from the face of a cell to the point where it enters the neighboring cell (optical path) and is measured as shown (Fig 6). The exponential scheme results in a negative value for radiative intensity for some of the test cases, which is physically incorrect [27]. In the second method, this situation is improved by approximating this distance to be the hydraulic diameter of the cell. This modification made to the exponential scheme was
validated using some benchmark test cases, and it was found that this modification helped to avoid the occurrence of negative intensity.

**Boundary Condition**

In general, to treat a boundary surface, a gray, diffuse wall boundary condition is considered as a good engineering approximation. In this RTE solver, all of the boundaries are assumed as gray diffuse boundaries, and the intensity at the boundary surface (wall) is calculated as

$$I_w = \frac{1-\varepsilon}{\pi} \int_{\hat{s},\hat{n}>0} I(s) \hat{n} \cdot \hat{n} d\Omega + \frac{k\sigma T_w^4}{\pi}$$

where

- $I_w$ is the intensity at the wall
- $\varepsilon$ is the emissivity of the wall surface
- $T_w$ is the wall temperature

**Treatment for Overhang Problem**

In the practical implementation of the FVM in the RTE solver using unstructured grids, the boundary of the control angles may not coincide with the boundaries of the control volume most of the times, as shown in Fig 7. This is the so-called overhanging problem. Under such circumstances, a numerical treatment is used to determine if the radiation is incoming or outgoing at that particular ray direction ($\hat{s}$). Many such over-hanging treatment techniques are available. This numerical approach uses one of the simplest approaches to handle this problem. It is called the bold approach [7, 35, 29].
The bold approach treats the overhanging control angle by assuming that the entire control angle is either incoming or outgoing at a cell face, depending on whether the mean direction $\hat{s}$ is pointing at or away from the face. This treatment is computationally less expensive and simple. In this approach, at each cell face, the solid angle of a ray associated with the direction $i$ is assumed to be outgoing to the cell if $\hat{s}.A > 0$, and is incoming otherwise.

**System of Linear Equations**

Following the discretization procedure explained before, a set of linear equations can be obtained that can be expressed as

$$a_pl_p = \sum_{nb} a_{nb}l_{inb} + b$$

(3.16)

where

- $l_p$ is the radiative intensity along direction $i$ in the cell center
- $l_{inb}$ is the radiative intensity along direction $i$ in the neighboring cells of the control volume surfaces
- $a_p$, $a_{nb}$ are the link coefficients of radiative intensity at the cell center and cell neighbor intensities
- $b$ is the source term
This equation expresses the cell center value of a cell in terms of its neighboring cells. If the total number of cells in the computational domain is $N_{\text{cell}}$ and the angular discretization is $N_0 \times N_\phi$, then this procedure leads to $N_{\text{cell}}$ equations in each of the $N_0 \times N_\phi$ directions. This $N_{\text{cell}}$ system of equations is solved simultaneously within each of the $N_0 \times N_\phi$ directions and the resulting radiative intensity $I_{ip}$ for a cell in every direction is summed over all directions, to get the total radiative intensity $I_p$ in that particular cell.

In this study, three numerical methods have been implemented to solve the system of linear equations. They are the Gauss Seidel method, the Under Relaxation method, and the Dynamic Under Relaxation method.

*Improvements to the FVM Solver*

Non-physical negative intensities occur in some test cases when the exponential scheme is employed. A modification to the system of equations based on suggestions from Patankar [38] has been implemented in this numerical approach. Calculation of the source term and the matrix coefficients has been modified to avoid the occurrence of negative intensities. For a 2D problem (Fig 6), the discretized set of equations, for a given direction $l$, can be written as

$$a_p^l I_p = a_{N1}^l I_{N1}^l + a_{N2}^l I_{N2}^l + b^l$$

(3.17)

where $a_p^l$ is the coefficient for the cell center

$a_{N1}^l, a_{N2}^l$ are the coefficients for the neighboring cell intensities and

$b^l$ is the source term.
The second term on the right-hand side of eq. (3.11) is generally treated as part of the source term for all of the cell faces. This term will be added as a negative source term for the faces whose upstream cell is the cell, P (i.e., for the faces e and n in this example). This sometimes results in a large negative source term, thus the solution procedure leads to a negative radiative intensity that is non-physical. To avoid this scenario, in the present approach, the second term of eq (3.11) is added to $a_p$ after dividing this equation by $I_{P0}$, where $I_{P0}$ is the radiative intensity at the centre of cell P calculated from the previous iteration. This approach is discussed in detail by Chai et al. [27], and Patankar [38] (Positive Coefficient Requirement).

**Full Spectrum Correlated-\( k \) Model (FSCK)**

The FSCK [32] is a global model that is based on extending the concept of reordering the \( k \)-distribution to the entire spectrum. This model uses the scaling approximation, i.e., the spectral and spatial dependence of the absorption coefficient obey the following relation [19],

$$
\kappa_{\eta}(\eta, T, p, \mathbf{x}) = k_{\eta}(\eta)u(T, p, \mathbf{x})
$$

(3.18)

where $\kappa_{\eta}$ is the raw absorption coefficient and $k_{\eta}$ is the spectrally dependent absorption coefficient.

As discussed in Chapter 2, instead of $k_{\eta} vs \eta$, $k(g) vs g$ can be used and the quadrature points obtained from $k(g) vs g$ can be used as the gray gases that can represent the non-gray gas. When this scaling approximation is introduced in the RTE, and the non-gray gas is represented by a mixture of gray gases, the resulting RTE is [19],

$$
\frac{dI_g}{ds} = ku a l_b - (ku + \sigma_s)I_g + \frac{\sigma_s}{4\pi} \int_{4\pi} I_g(\hat{s}')\phi(\hat{s}, \hat{s}') d\Omega
$$

(3.19)
where

\[ I_g = \int_0^\infty I_\eta \delta(k - k_\eta) d\eta / f(T_{ref}, k), \]

\[ a = f(T, k) / f(T_{ref}, k) \]

\[ k = k(T_{ref}, g_{ref}) \] is determined at some reference \( g \) and \( T \) and

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

This gray medium RTE has to be solved for a small number of gray absorption coefficients \( k(g) \) at the quadrature points, and the total intensity \( I \) is obtained by performing a weighted summation over the gray gas intensities, \( I_g \).

**Implementation of the FSCK model**

The implementation of the FSCK model involves the following steps.

*Forming \( \kappa \) (raw absorption coefficient) bins and computing \( f(T,k) \).*

i) A set of reference conditions must be chosen for a given case. This would include reference temperature, reference pressure, and reference species composition.

ii) For the chosen reference temperature \( (T_{ref}) \), the \( \kappa \) vs \( \eta \) plot must be generated at predefined uniform intervals of \( \eta \). In this study, \( \kappa \) has been generated from the spectroscopic database using the Lorentz line profile [8].

iii) The range of the absorption coefficient must be divided into a number of small intervals \( (J) \), called as \( \kappa \) bins. This number, \( J \), can be arbitrary. In a
study by Mazumdar et al. [39], 100 bins were taken for every 10 units of increment in κ.

iv) The bin values are initially set to zero. For every κ generated at $T_{ref}$ from step (ii), depending on whichever absorption coefficient interval it fits in, the corresponding bin value must be increased by the fractional Planck function ($I_{b\eta}$) computed at the corresponding $\eta$ value. These κ bins can be set up for several temperatures, and the increment to κ bins can be performed simultaneously.

v) Once step (iv) is completed, the sum of fractional Planck function values in the bins is multiplied by $\pi/\sigma T_i^4$ where $T_i$ is the temperature corresponding to the set of bins considered. Now the bin values represent

$$f(T, k_j)\delta k_j,$$

where $j$ is the $k$ bin index.

It is important to note that irrespective of the number of temperatures considered, the raw absorption coefficient value, κ is generated only at the reference temperature. For different temperatures, the difference comes in the Planck function value ($I_{b\eta}$) and thus $f(T, k_j)$ value.

Evaluation of weight function, $a$.

For evaluating the weight function $a$, first $k(T, g)$ must be determined. One of the simplest ways to determine $k(T, g)$ is shown as follows.

The $g$ function is calculated for each temperature as

$$g(T, k_j) = \sum_{j'=1}^{j} f(T, k_{j'})\delta k_j = g(T, k_{j-1}) + f(T, k_j)\delta k_j$$

(3.20)
This $g$ function now represents an equivalent Planck function. The weight function $a(T, g)$ is now determined by calculating the ratio of the slope of $g(T, k)$ to that of $g(T_{\text{ref}}, k)$. Once $k(g)$ is determined, a few quadrature points can be chosen in $k(g)$ vs $g$ for the integration of the RTE, as in eq. (3.19). In this thesis, Gauss Legendre and Gauss Jacobi quadrature schemes have been used to obtain the quadrature points. In previous studies by Mazumdar et al. [39], Gaussian quadrature of moments is recommended for obtaining quadrature points.

_Evaluation of scaling function, $u$._

Determination of a scaling function is a necessary step for problems involving inhomogeneous or non-isothermal conditions. The choice of a reference condition is very important in solving such problems. Some suggestions from Mazumdar et al. [39] and Modest et al. [19] in the choice of reference conditions are listed here.

_Choosing a reference condition_

The reference mole fraction distribution can be chosen to be the volume-averaged mole fraction distribution in the entire domain [19].

$$x_{\text{ref}} = \frac{1}{V} \int_V x dV$$

(3.21)

The reference temperature can be chosen in many ways, such as [19,39]

i. Hottest temperature in the domain.

$$T_{\text{ref}} = T_{\text{hot}}$$

(3.22)

ii. Coldest temperature in the domain.

$$T_{\text{ref}} = T_{\text{cold}}$$

(3.23)

iii. Planck mean temperature.
\[ T_{\text{ref}} = T_{\text{Planck}} \], which is computed from the relation

\[ (\kappa_p T^4)_{\text{Planck}} = \frac{1}{V} \int_V \kappa_p T^4 dV \]  

(3.24)

where \( \kappa_p \) is the Planck mean absorption coefficient and \( V \) is the volume of the domain. In this study, the values of Planck mean absorption coefficients used to determine the Planck mean temperature have been obtained from Zhang [40].

The emission weighted temperature can also be used as the reference temperature which is defined as

\[ T_{\text{ref}} = T_{\text{em}} = \frac{\int_V \left[ \kappa_p(T, p, x) T^4 \right] dV + \int_A \left[ \alpha T^4 \right] dA}{\int_V \left[ \kappa_p(T, p, x) T^4 \right] dV + \int_A [\sigma T^4] dA} \]  

(3.25)

where \( A \) is the area of the computational domain and 

\[ \sigma \] is the Stefan-Boltzmann constant.

From the experience gained from this study, \( T_{\text{Planck}} \) and \( T_{\text{hot}} \) are good choices for reference temperatures. They are also recommended in the previous studies [19,39].

**Computing mean beam length \( (L_m) \)**

Once the reference temperature and mole fraction have been found, the next step is to determine the mean beam length. Mean beam length determination varies for different problems and is computed as \( 4V/A \). Some guidelines to determine mean beam length for different problems have been listed in Reference 8.

**Computing scaling function \( u \)**

The scaling function \( u(T, p, x) \) can be evaluated by solving the following implicit relation with an assumption of constant total pressure throughout the domain [19].
\[
\int_0^{\infty} l_{bn}(T_{em}) \exp[-\kappa_n(T, x) L_m] d\eta = \int_0^{\infty} l_{bn}(T_{em}) \exp[-k_n u(T, x) L_m] d\eta
\] (3.26)

where \( k_n = \kappa_n(T_{ref}, x_{ref}) \)

To reduce the computational cost, it can be assumed that \( T_{em} = T_{ref} \). In this study, this equation is solved iteratively using the Newton-Raphson method for \( u \).

Angular Domain Decomposition-Based Parallel Algorithm

To improve the speed of calculations of the solver and to solve real-time problems within a reasonable time frame, parallel computing with domain decomposition is implemented in the present study. In radiative heat transfer calculations, three types of domain decomposition can be performed: spatial, angular, and frequency domain decompositions. Different types of domain decompositions and their comparative advantages and performance have been discussed in the literature [41,42]. In the current radiative solver, angular domain-based decomposition has been implemented, since it can achieve a linear speed up. In angular domain decomposition algorithm, the total number of control angles, \( N_\theta \times N_\phi \), can be equally divided among the number of processors. Each processor computes the total heat flux from all of the directions corresponding to the angle(s) assigned to it and sends the result to the master processor. The Message Passing Interface (MPI) library [43] is used in the implementation of parallel computing with angular domain decomposition.

A schematic diagram describing the implementation of this parallel computing algorithm is shown in Fig 8.
Figure 8. Schematic of the Parallel Algorithm.
CHAPTER 4
VALIDATION OF THE NUMERICAL APPROACH

The numerical procedure explained in chapter 3 is validated using standard test cases. These validation test cases are placed in three categories:

i. Validation of the gray gas RTE solver with constant absorption coefficients.

ii. Validation of the non-gray gas RTE solver for real gases using FSCK model for the absorption coefficient calculations.

iii. Study of the Parallel Performance.

Validation of the Gray Gas RTE Solver

This section presents the results of the validation of the Finite Volume Solver for test cases with a constant absorption coefficient. This validation involves testing the various capabilities of the solver, such as ability to handle unstructured meshes, and arbitrary geometries. Different test cases that are used to test the capabilities of the radiation solver are listed as follows.

Validation of the Gray Gas RTE Solver for Regular Geometries

The RTE solver is first validated for regular geometries such as square and cubic enclosures with and without participating medium. These test cases are discussed in the following sections.
Black Duct with No Participating Medium (2D)

The first test case [37] is a study of two-dimensional heat transfer in a square black duct (Fig 9a) without a participating medium. This is an important test case, because it demonstrates the ability of the radiation solver to handle test cases without a participating medium. The FVM performs best when there is a participating medium and the intensity varies smoothly in the angular direction. This test case is used to test the accuracy limitations of the FVM, as the absence of a participating medium results in sharp changes in radiative intensity, especially in the angular direction. A short description of the test case is as follows.

The computational domain consists of a unit square and is extruded in the third dimension by 10 units. The bottom wall of the square duct is held at a temperature $T_1$ (600 K) whereas all the other walls are held at $T_2$ (300 K). The heat flux at the top surface is non-dimensionalized as

$$q = \frac{q'}{\sigma(T_1^4 - T_2^4)}$$

(4.1)

where

$q'$ is the heat flux on the top wall.

This test case is studied extensively for various interpolation schemes (Fig 9b) and different spatial (Fig 9c) and angular mesh (Fig 9d) resolutions. Different mesh topologies are also used in this test case (Fig 9(e-g)). The exact solution for this test case is obtained from Raithby [37].

This test case was first analyzed for different interpolation schemes (step and exponential schemes) for a mesh resolution of (41x41). The results are plotted in Fig 9b. It is clear from the results that the choice of different interpolation schemes does not affect
the results for this test case. This is because the exponential scheme formulation reduces
to the step scheme in the absence of a participating medium.

A study was done to analyze the effect of spatial mesh resolution using this test
case. Three uniform spatial mesh resolutions (21x21, 41x41 and 71x71) are used in this
study. The results of this study are shown in Fig 9c. It can be concluded from this study
that the increase in the spatial mesh resolution improves the accuracy of the results. This
can be seen in Fig 9c, where the solution from higher mesh resolution (71x71 mesh)
shows better agreement with the exact solution than the solutions from lower mesh reso-
lutions (41x41 and 21x21 mesh).

Another study is conducted to analyze the effect of angular mesh resolution. Four
uniform angular mesh resolutions (2x16, 2x32, 2x64, and 2x112) are used in this study.
The spatial mesh resolution of 41x41 is used in this study. The results, from this study,
show that the oscillations in the heat flux values appearing in the case of lower angular
mesh resolution disappear as the mesh resolution is improved (Fig 9d). It can be co-
ncluded from this study that an increase in angular mesh resolution with a uniform spatial
mesh improves the accuracy of the results significantly.

This test case is also analyzed using different mesh topologies (orthogonal uni-
form mesh, orthogonal non-uniform mesh, and non-orthogonal uniform mesh). A com-
parison of the results for these different mesh systems is shown in Fig 9e. The orthogon-
al uniform mesh topology shows a smooth variation in heat flux, whereas the orthogonal
non-uniform mesh results in a solution that shows waviness in the heat flux distributions.
A sample plot of these two mesh topologies are shown in Fig 9(f,g) for a lower mesh res-
olution (21 x 21). It is also shown in the results (Fig 9e) that the solution from non-
orthogonal mesh shows a better agreement with the exact results as compared to other mesh systems. From this study it can be concluded that non-uniformity in the mesh systems highly affects the behavior of the solution of the radiative solver for test cases without a participating medium. A detailed study using non-orthogonal, unstructured mesh systems is discussed next.

A comparative study of different types of non-orthogonal, unstructured mesh topologies is conducted using this test case. A step (upwind) scheme with an angular discretization of $1 \times 24$ is employed to compute the radiative intensity in this mesh topology study. Two unstructured mesh systems are tested (Fig 9h and i). The numerical result, compared to the exact solution, are shown in Fig 9j. Though the numerical results with these two mesh systems are not exactly identical, the difference is very small, and both results compare well with the exact solution.

(a) Schematic Representation of the Computational Domain.

Figure 9. Black Square Duct with No Participating Medium.
Figure 9. Black Square Duct with No Participating Medium.

(b) Different Interpolation Schemes.  
(c) Different Spatial Meshes.  
(d) Different Angular Meshes.  
(e) Different Mesh Topologies.  
(f) Orthogonal Uniform Mesh.  
(g) Orthogonal Non Uniform Mesh.
(h) Non Orthogonal Mesh 1.  
(i) Non Orthogonal Mesh 2.

(j) Comparison of Different Unstructured Mesh Topologies.

Figure 9. Black Square Duct with No Participating Medium.
Black Duct with a Participating Medium (2D)

The second test case involves a two-dimensional heat transfer in a unit square black duct with a participating medium. In this test case, an absorbing emitting medium is maintained at a constant temperature of 300K, and the cold walls of the duct are kept at 0 K (Fig 10a).

A computational domain with 21x21 mesh points and an angular discretization of $1\times16$ is used in this study. This problem was previously reported by Chai et al. [27]. The absorption coefficient of the medium is maintained at $k = 10.0$ (optically thick medium). The results for this simulation are shown in Fig 10b, and 10c shows the difference in the predictions of the step and exponential schemes. The exponential scheme solution is slightly better when compared with the step scheme solution.

The same test case is also simulated using a non-uniform mesh using the step and exponential schemes. The exponential scheme shows a marginally better prediction (Fig 10c) when compared to the step scheme. The exact solution for this test case is obtained from Chai et al. [27].

(a) Schematic Representation of the Computational Domain.

Figure 10. Black Duct with a Participating Medium.
Different Interpolation Schemes

(b) Different Interpolation Schemes

(c) Different Interpolation Schemes in Non-Uniform Mesh.

Figure 10. Black Duct with a Participating Medium.

Black Enclosure with a Participating Medium (3D)

The ability of the radiative solver’s capability to handle three dimensional problems is validated using this test case. This case involves a three-dimensional heat transfer in a cubic duct [30] and is explained as follows.

A cubical enclosure of length $L_0$ (1 m) with black walls at 0 K (Fig 11a) is considered. The temperature profile in the enclosure is given by,

$$T(x,y,z) = \alpha T_0 h \left[ \frac{x - L_0/2}{L_0/2} \right] \left[ \frac{2(y - L_0/2)^2 + (z - L_0/2)^2}{L_0} \right] + (1 - \alpha)T_0$$  \hspace{1cm} (4.2)

where the function $h$ is given by,

$$h(p) = 1 - p^2$$  \hspace{1cm} (4.3)

The reference temperature, $T_0$, represents the peak temperature (300 K) in the enclosure. The parameter, $\alpha$, is for the steepness or non-uniformity of the temperature profile and is set to 0.5. In this case, an optical thickness of $KL_0 = 10$ is considered.
This test case is studied using a (15x15x15) computational mesh with an angular mesh of \((N_\phi = 12 \times N_\theta = 8)\). Fig 11b compares the predicted solution with the exact solution when \(kL_0 = 10\) at \(z = L_0\) and \(y = 0\); it can be seen that the numerical solution over-predicts the heat flux when compared to the exact solution. The exponential scheme heat flux prediction is in better agreement with the exact result than the step scheme heat flux prediction. To achieve an improvement in the results, the spatial mesh resolution is improved to 30x30x30, and the results with this higher mesh resolution are shown in Fig 11c. It can be seen from this Fig. that the exponential scheme solution matches well with the exact solution, and the results from the step scheme also show good improvement with a higher mesh resolution. From these results, it is clear that exponential scheme predictions are better than step scheme predictions for test cases with a participating medium. In addition, higher accuracies can be achieved in both step and exponential schemes by improving the spatial mesh resolution.

(a) Schematic Representation of the Computational Domain for the Test Case 3.

Figure 11. 3-D Black Duct with a Participating Medium.
Validation of the RTE Solver for Arbitrary Geometries with Unstructured Meshes

The capability of the radiation solver to handle tetrahedral and hexahedral meshes has been further validated. The RTE Solver has been tested with different 2-D and 3-D test cases with unstructured meshes, and the results are reported in this section.

Radiation in an Irregular Arc Geometry

The geometry for this test case [29,44] consists of a rectangle on top of a circular arc, as shown in Fig 12a. The curved wall is maintained at a higher temperature with an emissive power of unity. All of the other walls are cold and black. This test case was simulated for two conditions:

i. in the absence of a participating medium

ii. in the presence of a participating medium with the absorption coefficient, $k = 1 \text{m}^{-1}$
The result obtained from this simulation has been compared against the Monte Carlo solutions from Refs. 29, 44.

(a) Irregular Arc with Structured Mesh. (b) Comparison with Monte Carlo Method.

Figure 12. Radiative Heat Transfer on an Irregular Arc Geometry.

A structured spatial mesh of size 20×20, as shown in Fig 12a, and an angular mesh resolution of 4×16 are used in this calculation. The radiative heat flux on the right wall from the computation is presented in Fig 12b along with the results from Monte Carlo computations. It can be seen from the results that the computed solutions match well with the Monte Carlo solutions for both simulations, with and without a participating medium.

Radiation in a Rhombus Geometry

This test case simulates radiative heat transfer in a black rhombic enclosure (Fig 13a). The bottom wall is at a higher temperature with an emissive power of unity, and the other walls with the participating medium are at 0 K. The radiative heat flux at the top
wall is compared with the Monte Carlo solution available [29,44] in the literature (Fig 13b). It can be seen in this comparison that the results from the less expensive finite volume methodology adopted in this study compare very well with the Monte Carlo solutions, which are considered very accurate and computationally very expensive.

(a) Rhombus with Structured Mesh. (b) Comparison with Monte Carlo Method.

Figure 13. Radiative Heat Transfer on a Rhombus.

3-D Cylinder Geometry

A test case with a cylindrical computational domain with unit diameter and length of three units [36] is employed to test and validate the capability of the radiation solver in handling a 3-D computational domain with an arbitrary shape. The cylindrical domain is filled with a gray isothermal medium at a temperature of 1200 K, and the boundary is a black wall and held at 300 K. An unstructured tetrahedral mesh system consisting of 3955 cells used in this test case is plotted in Fig 14a. The mesh is considered to be very coarse. The net radiative heat flux at the side wall of the cylinder is calculated from the
radiative solver using the step scheme with a $2 \times 8$ angular discretization. Two different values of the absorption coefficient ($k$) for the participating medium have been chosen to represent weak (0.1 m$^{-1}$) and strong (10.0 m$^{-1}$) optical thicknesses. The results of these two conditions are compared to the solutions from ray method and plotted in Fig 14 (b,c), respectively. It can be seen that the radiative solver predicted the wall heat fluxes for both cases with reasonable accuracy. It should be noted that the waviness of the numerical results is caused by the variation of the radial distance at the center of each cell along the wall boundary. The non-uniformity of the radial distance is due to the combination of the coarse mesh and the nature of the unstructured meshes.

(a) Unstructured Tetrahedral Mesh on Cylindrical Enclosure.

Figure 14. Radiative Heat Transfer on a Cylinder
Radiation in a Tetrahedral Enclosure

Another test case with a tetrahedral enclosure (Fig 15a) is considered in this study to validate the capability of the radiative solver to handle arbitrary geometries. Each side of the tetrahedron is 1 m. The coordinates of the vertices of the geometry are given by (0, 0, 0), (1, 0, 0), (0.5, 0.866, 0), and (0.5, 0.288, 0.817). The walls of the tetrahedron are at a temperature of 0 K. The tetrahedron contains a medium at a temperature of 300 K ($T_{medium}$) and has an absorption coefficient ($k$) of 1.0 m$^{-1}$. This test case has been studied by Murthy et al. [35]. The computational domain is discretized using an unstructured mesh system consisting of 13,454 cells. This test case is analyzed with an angular discretization of 6×6. The dimensionless incoming heat flux is computed along a central line in one of the side walls (the line joining a side wall midpoint (0.75, 0.433, 0.0) and the vertex (0.5, 0.288, 0.817)). The results for both the step and exponential schemes are shown in Fig 15b. The plot shows the dimensionless heat flux,
\[ q = \frac{q^*}{\sigma T^4_{\text{medium}}}, \quad (4.4) \]

against the distance along the chosen line where \( q^* \) is the actual heat flux along the chosen line. The result shows a reasonable comparison with the exact results obtained from Murthy et al. [35]. As demonstrated earlier, in this test case (with participating medium), the exponential scheme shows a closer agreement with the exact solution than the step scheme.

(a) Tetrahedral Geometry. (b) Results for Tetrahedral Geometry.

Figure 15. Radiative Heat Transfer on a Tetrahedral Geometry.

Validation of the Non-Gray Gas RTE Solver

As discussed in Chapter 3, the capability to enable non-gray gas simulations has been introduced in this numerical methodology by the implementation of the FSCK model. This approach to simulate non-gray radiation is validated with several test cases. Some of the test cases are discussed in this section.
Spectroscopic Databases

All of the computations discussed in this section have been calculated using the spectroscopic database, HITEMP. The structure of the HITEMP database is similar to that of the HITRAN database [45] and is considered to be accurate when used up to a maximum temperature of about 1500 K.

Isothermal and Homogeneous Test Case

The first test case [39] considered for this study is under isothermal and homogeneous conditions. It is claimed that the only approximation in the FSCK model is the scaling assumption, which is employed under non-isothermal and inhomogeneous conditions [19, 39]. Thus, for a homogeneous and isothermal test case, the FSCK model should produce accurate results. To verify this claim, the FSCK model implementation is tested with an isothermal and homogeneous test case. In this test case, a layer of 10% CO$_2$ and 90% N$_2$ gas is trapped between two black parallel plates at a temperature of 1500 K (Fig 16a). The plates are maintained at 0 K and are 1 m apart. This test case is simulated with a spatial mesh resolution of 40 cells across the y-direction and an angular mesh resolution of 4x16 ($N_\theta \times N_\phi$). The divergence of heat flux across the gas layer is plotted in Fig 16b, and the local radiative heat flux across the gas layer for this simulation is plotted in Fig 16c. It can be seen from these results that the computations are very accurate for this isothermal and homogeneous test case. In addition, a grid sensitivity study has been done by repeating the calculation with a higher spatial mesh resolution (80 cells in the y-direction) first and with a higher angular mesh resolution (4×32) next. Good accuracies in the results are achieved by using these higher mesh resolutions, although the difference from
the original mesh results is very small. It is also of interest to study the effect of optical thickness in the accuracy of the results. Hence the test case is simulated for smaller optical thickness (optically thin medium) by changing the distance between the parallel plates to 1 cm. The divergence of radiative heat flux and the local radiative flux in the gas layer between the plates has been computed for this optically thin medium simulation and compared with the line-by-line calculation results (Fig 16c and e) available in the literature [39]. It can be seen from these results that the accuracy slightly reduces as the medium becomes optically thinner, especially near the boundaries. It can be concluded from these results that the FSCK model with the FVM framework produces accurate results for isothermal and homogeneous conditions, especially under optically thick situations.
T(wall) = 0K

CO₂ at 1500 K

(a) Schematic of Isothermal, Homogeneous Test Case.

(b) Divergence of Heat Flux (L = 1m).

(c) Divergence of Heat Flux (L = 1cm).

d) Local Heat Flux (L = 1m).

e) Local Heat Flux (L = 1cm).

Figure 16. Isothermal, Homogeneous Test Case.
Non-Isothermal and Homogeneous Test Case

As discussed earlier, the only assumption in the FSCK model is the scaling approximation. This assumption is effective under non-isothermal or inhomogeneous conditions. To check the limitations of the FSCK model, it is important that this model be tested under non-isothermal or inhomogeneous conditions. This non-isothermal test case with a sudden drop in temperature in the domain is used to check the accuracy limitations of the FSCK model and the effect of the scaling approximation employed.

In this test case [39], a mixture of (10% CO$_2$ and 90% N$_2$) gas between two parallel plates is considered. There are two layers of this gas mixture at hot and cold temperatures, with a temperature discontinuity existing between these two layers (Fig 17a). The hot gas layer is at a temperature of 1500 K ($L_{\text{hot}}$), and the cold gas layer is at a temperature of 500 K ($L_{\text{cold}}$). The plates are considered black and are maintained at a temperature of 300 K. The thickness of the hot layer is maintained at 50 cm. The test case is simulated under three different conditions by changing the thickness of the cold layer (keeping the hot layer thickness as 50 cm) as follows.

i. $L_{\text{hot}} = 50$ cm and $L_{\text{cold}} = 25$ cm

ii. $L_{\text{hot}} = 50$ cm and $L_{\text{cold}} = 50$ cm

iii. $L_{\text{hot}} = 50$ cm and $L_{\text{cold}} = 150$ cm

This is a difficult condition to simulate in terms of scaling assumption, due to the abrupt temperature drop of 1000 K between the hot and cold layers. This case thus serves as a test for the scaling approximation used in the FSCK model.
Simulation under condition (i). In this study, a 25cm thick cold layer is considered. To represent the $k$-distribution, a Gauss Legendre scheme with 10-point quadrature is used. This test case is simulated with a spatial grid of 40 cells and an angular grid of 4x16. The results show good comparison with the LBL solutions except at the hot layer region (Fig 17b). From Fig 17b, it can be seen that the divergence of the heat flux in the hot temperature layer is slightly over predicted when compared to the results from the LBL simulation obtained from Reference 39. The divergence at the cold layer matches well with the LBL results. Improving the spatial grid resolution to 80 cells does not improve the solution significantly. Another study with an improved angular grid resolution of 4x32 shows that there is not much improvement in the accuracy of the solution, especially in the hot temperature layer.

Simulation under condition (ii). In this study, a cold-layer thickness of 50mm is considered. To represent the $k$-distribution, a Gauss Jacobi scheme with 15-point quadrature is used. This test case is simulated with a spatial grid of 40 cells and angular grid of 4x16. For this simulation, the results show a good match with the LBL calculations [39]. This study is repeated with improved spatial grid resolution of 80 cells, and the results (Fig 17c) do not differ much from the original grid (40 cells). Improving the angular grid resolution also does not affect the results significantly (Fig 17c).

Simulation under condition (iii). In this study, a cold-layer of 150 cm thick is considered. To represent the $k$-distribution, a Gauss Legendre scheme with 10-point quadrature is used. This test case is simulated with a spatial grid of 40 cells and an angular grid
of 4x16. The results (Fig 17d) show that the divergence of heat flux is overpredicted at the hot layer region compared to the LBL predictions. To study the effect of the number of quadrature points, another set of simulations are made with 30 quadrature points. It can be seen from the results (Fig 17d) that, with 30 quadrature points, the predicted divergence of heat flux matches well with the exact solution. Improving the angular grid resolution with 30 quadrature points does not make much difference in the results. Increasing the spatial grid resolution to 80 cells increases the divergence of heat flux at the location of temperature discontinuity. This is expected because when there is a discontinuity in the temperature, there is a discontinuity in the heat flux, and the divergence tends to infinity at that location.

From this study, it can be concluded that the FSCK model handles the presence of temperature discontinuity with reasonable accuracy. Increasing the number of quadrature points improves the accuracy of the solution significantly. Use of suitable quadrature schemes that best represent the $k$-distribution can improve the accuracy of the solutions obtained for non-isothermal test cases. For example, the Gaussian quadrature of moments is considered to be best suited to represent the $k$-distribution for some cases [39].
Figure 17. Non-Isothermal, Homogeneous Test Case.
**Non-Isothermal Parabolic Temperature Profile**

This test case contains 10% CO\(_2\) gas contained between two parallel plates with a parabolic temperature profile. The temperature distribution \(T\) is represented by the equation.

\[
T = T_c - (T_c - T_w) \left(\frac{2y}{L} - 1\right)^2
\]

(4.5)

where \(T_c\) is the temperature at the center

\(T_w\) is the wall temperature (500 K)

\(y\) is the distance from the bottom plate and

\(L\) is the distance between the two plates (1 m)

Two different temperature distributions with \(T_c = 1000\) K and \(T_c = 1500\) K are studied in this test case. The test case represents realistic scenarios such as combustion applications where the temperature varies gradually over a small interval. The results from the simulation where \(T_c = 1000\) K and the temperature gradually varies to \(T_w = 500\) K at the wall are plotted in Fig 18a. It can be seen from this plot that the predicted divergence of heat flux matches well with the LBL calculations [40]. In this simulation, a spatial mesh with 60 points across the gas layer to represent the temperature variation is used, and 15 quadrature points are used in the FSCCK model. For the reference temperature, the Planck Mean Temperature (850 K) is used.

The results from the simulation where \(T_c = 1500\) K is plotted in Fig 18b. It can be seen that there is a notable discrepancy in the results when compared to the LBL calculations. In this simulation, 60 spatial mesh points are used to represent the temperature distribution and 15 quadrature points are used in the FSCCK model. For the reference temper-
nature, the Planck Mean Temperature (1205 K) is used. The reasons for this difference in the results may be due to

i. an inadequate number of quadrature points (15) used to represent the $k$-distribution.

ii. an inadequate spatial mesh resolution (60 points to represent the temperature distribution).

This test case requires further study. It is expected that the accuracy of the results can be improved with an increase in the number of quadrature points.

(a) Divergence of Heat Flux, $T_c = 1000$ K. (c) Divergence of Heat Flux, $T_c$=1500 K

Figure 18. Test Case with Parabolic Temperature Profile.

Parallel Performance

The parallel performance of the angular domain-based parallel algorithm implemented in this approach is verified in this study. A cubical black enclosure with a gray participating medium discussed in the validation of gray gas simulation (Test Case 3) is used in this study. To study the parallel performance, a spatial mesh of $15 \times 15 \times 15$ and an
angular mesh of 8×12 is used. If the time taken for this test case with the serial algorithm is taken as \( t_s \), and the time taken by number of processors \( n \) is \( t_{np} \), then the speed up is defined as \( \frac{t_s}{t_{np}} \). It was verified for all of the simulations that the results obtained from the parallel computations matched the results obtained from the serial algorithm. A plot of speed up vs. the number of processors for this test case is shown in Fig 19 in comparison to the ideal linear speed up. From this figure, it is clear that the parallel algorithm based on angular domain decomposition shows good speed up characteristics (about 80% speed up with 12 processors) for the given test case. In addition, the algorithm using MPI REDUCE slightly outperforms the algorithm using MPI ISEND – RECV for these computations.

![Figure 19](image-url)

Figure 19. Parallel Performance (Speed up vs. Number of Processors).
CHAPTER 5
CONCLUSIONS AND FUTURE WORK

This chapter summarizes the conclusions from this study and discusses the further work required.

Conclusions Based on Present Study

Due to the complexity and cost involved in the experimental and analytical study of radiative heat transfer, especially in re-entry vehicle applications, a numerical approach is preferred. A numerical methodology for modeling radiation has been discussed in this report, based on the FVM for solving the governing RTE and FSCK models for spectral integration. This methodology has many advantages, specifically in terms of computational cost, ease of integration with CFD Solvers, and accuracy.

The validation of the implemented methodology is discussed in Chapter 4. The FVM has been validated first using gray gas test case conditions and found to be reasonably accurate. From the grid sensitivity study, it can be concluded that the accuracy of FVM can be improved by increasing the spatial and angular grid resolutions. From the results of the test cases with a participating medium, it is clear that the exponential scheme predictions are more accurate than the step scheme predictions.

For the validation of the FSCK model, test cases with real (non-gray gas) species have been used. The FSCK model gives accurate results for isothermal and homogeneous test cases. For non-isothermal test cases, the FSCK results can be improved by choosing
the right choice of reference temperature and by increasing the number of quadrature points. Numerical experiments showed that the Planck Mean Temperature can be considered as a good choice for reference temperature for test cases with non-isothermal conditions.

A parallel algorithm based on angular domain decomposition is implemented, and it has been shown that a good speed up can be achieved with this algorithm.

Future Work

The present work is a part of the development of computational tools that can aid in the simulation of radiative heat transfer in re-entry applications. To achieve this goal, more work need to be done in the following areas.

The capability to simulate scattering must be incorporated in the radiative solver. In the re-entry vehicle applications, there can be the presence of heat shield particles in front of the nose of the vehicle during re-entry. This can result in significant scattering of radiative heat. Hence this capability is important in terms of re-entry applications. More sophisticated boundary conditions (e.g., symmetry boundary) must be implemented in the present solver.

The validation of the FSCK model has been done for isothermal and non-isothermal non-gray conditions up to a temperature of 1500 K with CO$_2$ species. Further validation with a mixture of gas species and for higher temperatures needs to be done. To achieve this, the availability of high temperature databases for different species of air mixture should be explored. Currently, a Lorentz line profile is used to compute the absorption coefficient from a spectroscopic database, but this needs to be modified to voight
profile computations, since it is more appropriate to use the voigt profile [5,8,46] in high
temperature applications where the Doppler effect is also important.

The FSCK model must be further improved to a Multi Group/Multi Scale FSCK
model or further upgraded models to handle non-homogeneous, high temperature appli-
cations accurately.

The developed RAD-FVM model must be coupled with CFD to account for the
change in temperatures and species concentration for high temperature applications. Spa-
tial domain-based parallel algorithm to handle large test cases has to be implemented.
LIST OF REFERENCES


APPENDIX A

USER MANUAL FOR THE FINITE VOLUME GRAY GAS SOLVER
This appendix serves as the user manual for the FVM-based gray gas radiation solver. The information about the input and output files are listed in this section.

INPUT FILES

The FVM-based gray gas solver uses three input files, as follows

i. Case Name File (Define.dat)

ii. Grid File (case name.grd)

iii. Case File (case name.vars)

Case Name File

The case name file contains the name of the case that is to be simulated. This file is always named as ‘Define.dat’.

Grid File

The grid file contains information about the geometry and the computational grid to be used in the simulation. The information in the grid file should adhere to the following format.

i. dimensions : This line contains the information about the dimension of the test case. The dimension of the test case should be mentioned as ‘2D’ or ‘2d’ for a 2-D test case and ‘3D’ or ‘3d’ for a 3-D test case.

ii. nboundaries : The number of boundaries or boundary conditions in the test case is listed next.
iii. \( xL, yL, zL \): This line contains the information about the maximum length of the domain in \( x \), \( y \), and \( z \) directions.

iv. \( nc, nf \): This line contains information about the total number of cells \((nc)\) and total number of faces \((nf)\) in the computational domain.

v. \( xc, yc, zc \) (nc lines): The next nc lines list the \( x \), \( y \), and \( z \) cell center coordinates of all of the cells in the computational domain.

vi. \( v \) (nc lines): The following nc lines contain the values of volume of all the cells.

vii. \( ncf \) (nc lines): The next nc lines contain information about the number of cell faces of all of the cells listed sequentially.

viii. \( a \) (nc x nf lines): The area information for all of the faces of each cell is listed sequentially for the next nc x nf lines.

ix. \( n1, n2, n3 \) (nc x nf lines): The normal vectors in terms of their \( x \), \( y \), and \( z \) coordinates is listed sequentially for the next nc x nf lines.

x. \( nb \) (nc x nf lines): The following nc x nf lines contain the neighbor cell number for all the faces, for all of the cells.

xi. face_xc, face_yc, face_zc: The \( x \), \( y \), and \( z \) co-ordinates for the face centers for all of the faces is listed next in the grid file. This information is required only when the exponential scheme is used for the computations. The step scheme computations do not need this information.
Case File

The case setup information, including the boundary conditions, the spatial schemes used, and the properties of the medium are all listed in the case file.

The parameters required in this file can be grouped into divided into five groups. The case file contains the test case information in the following order of namelists.

i.  Medium Parameters

This name list contains the following information in the same order as listed as follows:

1.  absorp : The absorption coefficient of the medium. In case of a non-participating medium, the value is zero. In case of a non-gray medium, a dummy value is given for this coefficient.

2.  scat : The scattering coefficient of the medium. In case of a non-scattering medium, this value is zero.

3.  Scattering : If scattering is present the character ‘y’ is used; otherwise ‘n’ is used to indicate no scattering.

4.  temp_distribute : Temperature distribution in the medium. If this values is 0, then the temperature values are read from a file, Temp.dat. If this value is 1, then the medium temperature is a constant given by the value of the next parameter, medium_temp. If the value is 2, then the temperature is defined by a function and the function need to be included in the subroutine “TemperatureFunction”, under the module “ICand BC.f90”.

5. medium_temp : The value given here is assigned as the temperature of the medium, if temp_distribute value is 1.

ii. Boundary Conditions

This namelist contains the following boundary condition parameters.

1. nsurf : The number of boundary surfaces.
   The following conditions are listed for (nsurf) all of the boundary surfaces.

2. wtemp : boundary wall temperature.

3. wall_type : Boundary wall type, ‘b’ for black wall and ‘g’ for gray wall.

4. Emvst : The value of emissivity for the boundary wall, it is always 1 for black wall.

iii. Solver Parameters

The solver set up is governed by this parameters.


iv. Angular Grid Parameters

These parameters govern the angular discretization.

1. solid angle : There is only one choice of solid angle available, i.e., a uniform solid angle, indicated as ‘u’.

2. ntheta : Number of angles in the azimuthal direction.

3. nphi : Number of angles in the polar direction.
4. overhang_treatment : An ‘y’ indicates overhang treatment is required and an ‘n’ indicates that it is not required.

v. Case Parameters

These parameters govern the output of the RTE Solver.

1. ref_temp1, ref_temp2 : The heat flux output from the FVM Solver is non dimensionalised by dividing by the difference in emissive powers of ref_temp1 and ref_temp2.

2. axis : a value of ‘x’ indicates that the x axis co-ordinate will be printed with the output; similarly ‘y’ and ‘z’ would indicate y and z axis co-ordinates, respectively, and ‘a’ would indicate that all x, y, and z would be printed.

Output Files.

One output file is generated for each boundary surface. The name of the output file will be the case name followed by the word ‘Result’ followed by the boundary number and, finally, the filename extension ‘.dat’. For example, if the case name is ‘test’, then the output file for the first boundary will be named as ‘testResult1.dat’. The values of heat flux at the corresponding boundary cells with the x, y, and z co-ordinates are printed in the output file. If heat flux values are required at any other location that is not a boundary, then the subroutine ‘HeatFlux.f90’ must be modified accordingly to generate the results at the required location.

The program can be run by executing the command ‘FVM3D_intel’
APPENDIX B

USER MANUAL FOR THE FSCK MODULE
This appendix contains information about the input and output files for the FSCK module.

INPUT FILES

The following input files are required by the FSCK module.

i. fskdist

ii. scale

‘fskdist’ File

This file contains information required to generate the $k$-distribution in the FSCK module. This file contains the following information in the following order.

1. nmol : Number of species in the gas mixture.

2. xmfr, molemass : the species molefraction and molecular mass of the species shouldn't be listed for all of the species.

3. ipl, Tref, P: choice of absorption coefficient. $ipl = 0$ generates linear absorption coefficient, and $ipl = 1$ generates a pressure-based absorption coefficient. $Tref$ is the reference temperature. $P$ is the total pressure in the domain.

4. numT : number of temperatures for which the $a$ and $u$ value needs to be generated.

5. nq : number of quadrature points.

6. $T$ (numT lines) : All the numT temperature values are listed.

7. spect : the name of the spectroscopic database file.
8. wvnm_b, wvnm_e, wvnmst : the minimum, maximum wavenumber to be considered for the analysis and the increment in wavenumber to be considered for the construction of the absorption coefficient plot.

’scale’ File

This file contains the input parameters required to calculate the scaling function ‘u’.

1. n1000 : total number of lines in the absorption coefficient file.
2. lm : mean beam length value.
3. de : wavenumber interval for the absorption coefficient file.
4. Tref : Reference temperature for the calculation of scaling function, u.

OUTPUT FILES

The FSCK module generates the following output files.

i. kvsg.dat
ii. u.dat

‘kvsg.dat’ File

This file contains the nq lines for nq quadrature points and has the following information listed in the given order for all of the quadrature points.

1. Absorption coefficient value ‘k’
2. ‘g’ value for all the numT temperatures, which is explained in Chapter 3.
3. ‘a’ value for all the numT temperatures, as explained in Chapter 3.
‘u.dat’ File

This file contains the following information in the order listed below for numT temperatures.

1. T : temperature value.
2. u : scaling function value.

The program can be run by executing the command ‘fskdist’