A Hybrid Discrete Ordinates - Spherical Harmonics Method for Solution of the Radiative Transfer Equation in Multi-Dimensional Participating Media

A Thesis

Presented in Partial Fulfillment of the Requirements for the Degree Master of Science in the Graduate School of The Ohio State University

By

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ABSTRACT

The Radiative Transfer Equation (RTE) is a multi-dimensional integro-differential equation. It is difficult to obtain an exact analytical solution to the RTE even for simple one-dimensional cases due of its directional nature. As a result, approximate numerical methods must be used to solve the RTE. The two most popular methods that are currently used to solve the RTE are the Method of Spherical Harmonics ($P_N$ approximation) and the Discrete Ordinates Method (DOM or $S_N$ approximation). However, neither of these methods exhibit good accuracy over the entire range of optical thickness of practical interest. The $P_N$ approximation, although it shows good accuracy for optically thick regimes, it is not accurate for optically thin media and in scenarios in which radiation propagation is strongly directional, such as that of a medium bounded by a combination of hot and cold walls. The $S_N$ method, on the other hand, does show promising accuracy over a wide range of optical thickness. However, it suffers from ray effects in optically thin media, resulting in locally unphysical solutions. In optically thick media, the strongly coupled directional equations in DOM, renders the method computationally very expensive for obtaining accurate results. Keeping in mind the advantages of each of the afore-mentioned methods and the regimes in which they are accurate, a new robust and computationally efficient hybrid method that has acceptable accuracy over a wide range of optical thickness is proposed, developed, and demonstrated in this thesis.
The philosophy of splitting of radiant intensity as used in the Modified Differential Approximation (MDA) is employed here. This philosophy was originally proposed to remove the shortcomings of the $P_1$ approximation in optically thin media. The radiant intensity is split into two components, namely a “ballistic” (wall-emitted) component, and a “diffuse” (medium-emitted) component. Traditionally, the ballistic component is determined using a combination of view-factor based surface-to-surface exchange relations and ray-tracing algorithms, and the diffuse component is determined by invoking the first order spherical harmonics ($P_1$ approximation). Though this method has been shown to be accurate over a wide range of optical thickness, recent studies have shown that this method is prohibitive both from a memory and computational efficiency standpoint for complex three-dimensional geometry with obstructions. The inefficiency stems from the use of the view-factor based approach for determination of the wall-emitted component. In the new hybrid method proposed here, the “wall” component is computed using the Control Angle Discrete Ordinates Method (CADOM), a variant of the Discrete Ordinates Method (DOM), and the “medium” component is evaluated invoking the $P_1$ approximation. This hybrid $S_N - P_N$ method was validated for both two-dimensional (2D) and three-dimensional (3D) geometries against benchmark Monte Carlo results for gray media in which the optical thickness was varied over a large range. In all cases, the accuracy of the hybrid method was found to be within a few percent of Monte Carlo results, and comparable to the solutions of the RTE obtained directly using CADOM. As a noteworthy advantage, this method was found to be nearly 100 times more efficient than standalone CADOM in optically thick gray media. To demonstrate the method further, 3D non-gray calculations were performed for a gaseous medium with the wide-band model for
spectral properties, and the hybrid method was again found to provide substantial computational gains over standard CADOM.
Dedicated to my family for their never-ending love and support
ACKNOWLEDGMENTS

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<td>Area of face $f$ [m$^2$]</td>
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<td>$\Delta A$</td>
<td>Elemental area [m$^2$]</td>
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<td>$G$</td>
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<td>Cavity width [m]</td>
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<td>$J$</td>
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<tr>
<td>$M$</td>
<td>Number of boundary faces</td>
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<tr>
<td>$N_c$</td>
<td>Total number of cells in the computational domain</td>
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<tr>
<td>$N_{dir}$</td>
<td>Number of discrete ordinates (or directions)</td>
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<td>$q_{rad}$</td>
<td>Radiative heat flux [W m$^{-2}$]</td>
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<tr>
<td>$q_{cond}$</td>
<td>Conductive heat flux [W m$^{-2}$]</td>
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<td>$q_w$</td>
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<td>$q_m$</td>
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CHAPTER 1

INTRODUCTION

1.1 Background

Thermal radiation refers to a mode of heat transfer caused by electromagnetic waves between 0.1 $\mu$m to 10 $\mu$m in wavelength. Unlike the other two modes of heat transfer - conduction and convection - that depend on the first power of temperature, radiative heat transfer scales as the fourth power of the absolute temperature. Consequently, radiation becomes the dominant mode of heat transfer in high temperature applications, such as combustion, propulsion, rapid thermal chemical vapor deposition, chemical processing reactors, engines, and gas turbines to name a few. Another distinctive feature of radiation is that there is no medium necessary between two points for radiative heat transfer. This essentially makes radiation the only means of heat transfer in space or vacuum, e.g., in dissipation of heat and in cooling of power systems in outer space. The wide range of potential applications provides strong motivation for continued research in the field of radiative heat transfer.
Especially in combustion applications, either for power production or propulsion, consideration of thermal radiation becomes extremely important because the combustion process, as well as the heat transfer rates, are greatly influenced by radiation. Although radiation remains the dominant mode of heat transfer in these applications, conduction and convection also have to be considered for evaluating the total heat transfer rate. Thus, in the solution of any high temperature flow problem which involves all three heat transfer modes - conduction, convection, and radiation, apart from the usual challenges encountered due to solution of a number of conservation equations for the conductive and convective parts of the problem, a greater complexity now arises due to the difficulty faced in evaluation of the extra radiative heat flux term that appears in the general equation for energy conservation.

For a typical high-temperature application, the general equation for energy conservation, including all three modes of heat transfer, can be expressed as

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho U h) = -\nabla \cdot q + S_h$$

(1.1)

where \(\rho\) is the density of the fluid, \(h\) is the enthalpy, \(U\) is the fluid velocity and the heat transfer rate \(q = q_{\text{cond}} + q_{\text{rad}}\). The terms on the left side of the equation represent transport of enthalpy by the fluid. The first term on the right side represents the contribution to energy transfer as a result of conduction and radiation, and the second term represents an external heat source or external work done. Even though the radiative heat flux is just part of the total heat flux term in Eqn. 1.1, it is difficult to evaluate, particularly in the case of participating media. This divergence of the radiative heat flux term that appears in the overall energy equation is an unknown
and has to be determined separately from the equation of conservation of radiative energy in order to attain closure.

Radiation transport involves transport of a quantity, known as the radiant intensity, $I$, that is a function of 7 independent variables, viz., three spatial coordinates, two angular coordinates describing the direction of photon travel, the wavelength of radiation and time. This fundamental variable, $I$, is defined as follows.

$$I_\lambda(r, \hat{s}) = \lim_{\Delta A \to 0} \frac{\Delta Q_\lambda}{\Delta A}$$  \hspace{1cm} (1.2)

where $\Delta Q_\lambda$ represents the spectral directional radiant energy rate that passes through an elemental area $\Delta A$, per unit solid angle and per unit wavelength. This element is perpendicular to the ray direction $\hat{s}$ and has its center at $r$. In general, the intensity varies in an infinitesimal solid angle $d\Omega$ that lies in the direction $\hat{s}$, and the Radiative Transfer Equation (RTE) governs this variation.

The general Radiative Transfer Equation is written as [1]

$$\frac{1}{c} \frac{\partial I_\lambda}{\partial t} + \hat{s} \cdot \nabla I_\lambda = \kappa_\lambda I_{b\lambda} - (\kappa_\lambda + \sigma_{s\lambda})I_\lambda + \frac{\sigma_{s\lambda}}{4\pi} \int_{4\pi} I_\lambda(\hat{s}_i)\Phi_{s\lambda}(\hat{s}_i, \hat{s})d\Omega_i$$  \hspace{1cm} (1.3)

where $c$ is the speed of light, $\kappa_\lambda$ is the spectral absorption coefficient, $I_{b\lambda}$ is the black body intensity (or Planck function) and $\sigma_{s\lambda}$ is the spectral scattering coefficient. In this equation, the two terms on the left-hand side represent the temporal variation of the intensity and its transport through space. The first term on the RHS represents augmentation due to emission by the medium, and the second and third terms denote attenuation through absorption and out-scattering, respectively. The fourth term is the in-scattering term accounting for the increase in intensity because of the diverted
photons from the other solid angles into $d\Omega$. The scattering phase function is denoted
by $\Phi_{s\lambda}(\hat{s}_i, \hat{s})$ and physically represents the probability of radiation scattering from the
solid angle $d\Omega_i$ (in the $\hat{s}_i$ direction) to the solid angle $d\Omega$ (in the $\hat{s}$ direction).

Although the governing equation for radiation transport is known, it is difficult to
solve. This difficulty is primarily because of the fact that the RTE is a 7-dimensional
integro-differential equation with the radiant intensity depending on all 7 variables.
In most cases, these dependencies are also not straightforward. For instance, the
spectral behavior of gases is a really strong function of temperature and wavelength.
For correct predictions, the line spectra of gases must be accurately represented across
the entire spectral range. In inhomogeneous participating media, the intensities in
different directions get coupled, making the accurate computation of these intensi-
ties quite cumbersome. Thus, a combination of the above complexities makes the
analytical solution of the problem a challenging task. Hence, there has always been
the quest for the development of robust, accurate, general-purpose and efficient com-
putational methods for predicting radiative heat transfer rates in practical systems.
In the following section, the existing methods of solution of the RTE will be criti-
cally discussed. Following this discussion, the rationale for the current work will be
presented.

1.2 Computational methods used for modeling radiation

Despite the high degree of complexity involved in solving the RTE, a number of
numerical techniques exist in the literature for the determination of radiative heat
transfer rates in various engineering geometries with participating media. As real
problems are almost always of a conjugate nature, according to Howell [2], any pratical numerical method should have the following features.

- Capability to handle multi-dimensional and complex geometry.
- Good accuracy under all conditions - Varying degrees of scattering by the media, gray and non-gray, participating media.
- Ease of application
- Availability of the accurate intensity and the integrated quantities.
- Computational compatibility with Computational fluid dynamics (CFD) codes
- Low computational cost

A number of researchers have worked on developing methods aimed at achieving the above criteria. This section will provide a brief overview of the existing methodologies used to date. Detailed discussion of the existing methods in radiation can be found in Modest [1]. These methods have traditionally been adopted from the neutron transport field, and modified to suit radiation transport.

1.2.1 Exact Analytical Method

Analytical methods can be applied to radiative heat transfer problems only in the case of highly idealized situations, such as problems with simple geometry and homogeneous participating media having spectrally independent radiative properties. For example, the RTE applied to one-dimensional plane parallel media have abundant
applications in various fields, such as atmospheric sciences, neutron transport, etc. The reader is referred to [1] for the exact analytical solutions for these simple cases. Over the years, Crosbie et. al. [1] have provided exact formulations of the RTE for the case of absorbing-emitting-anisotropically scattering media for one dimensional cases. However, for complex radiation problems with inhomogeneous participating media and spectrally dependent radiative properties, obtaining the exact analytical solutions of the integro-differential RTE is exceedingly difficult. Therefore, for such complicated problems, approximate numerical methods are necessary. Nevertheless, exact analytical solutions are useful in providing quantitative indications for more difficult problems and serve as benchmarks against which other approximate numerical methods can be validated.

Amongst the different numerical methods that have been developed thus far in this field, a popular means of classification of them is stochastic and deterministic. Of the stochastic methods, the Monte Carlo is the most popular technique that is discussed in the following section.

### 1.2.2 Monte Carlo

The Monte Carlo method is a stochastic method that can simulate relevant physical processes with relative ease and with high accuracy. In the context of radiation transport, it is amenable to addressing physics such as strongly varying spectral properties, directional surface properties, amongst many others. Problems in radiation are particularly well suited to solution by a Monte Carlo technique since energy travels as discrete parcels (photons) along a straight path before interaction with matter.
Solving a thermal radiation problem using the Monte Carlo technique implies tracing the history of a statistically meaningful sample of photons from their points of emission to their points of absorption. A detailed discussion of this technique may be found in Modest [1]. Unfortunately, since the method is stochastic, a large number of statistical samples are often needed to attain high accuracy rendering the method computationally very expensive. Furthermore, the results of a Monte Carlo calculation have inherent statistical errors that cannot be completely eliminated. On account of these shortcomings, it is fair to conclude that while the Monte Carlo method is desirable for the generation of benchmark solutions for relatively simple problems, it is prohibitively expensive and/or intractable for large-scale three-dimensional geometries as encountered in the simulation of practical engineering devices. Moreover, because of the stochastic nature of the method, it is difficult to couple the Monte Carlo RTE solver with deterministic flow solvers.

1.2.3 Zonal Method

The Zonal method, a method first developed in the 1950’s by Hottel and Sarofim [3], is a method in which the enclosure is divided into a finite number of isothermal volumes and surface area zones. Each element is assumed to have a uniform temperature distribution and radiative properties. An energy balance is performed for calculating the radiative exchange between any two zones, employing some pre-calculated “exchange factors”, that are defined similar to those defined for surface to surface radiation exchange. This process leads to a set of simultaneous equations for the unknown temperatures or heat fluxes. Later, Yuen and Takara [4] extended
this idea to a general zonal method for analysis of radiative transfer in absorbing and anisotropically scattering media. Some of the inherent limitations of this method, as pointed out by Hottel and Cohen [5], is the treatment of non-gray and temperature dependent radiative properties. If the radiative properties are temperature dependent, the exchange factors have to be recalculated over and over again as the temperature is calculated iteratively. Also, for complex 3D geometries, the computation and storage of volumetric exchange factors is computationally very expensive and this method can be completely prohibitive if refined grids are used for the computations [6].

1.2.4 Method of Spherical Harmonics

The spherical harmonics method or $P_N$ approximation uses a series approximation for the angularly dependent intensity field to replace the integro-differential RTE with a set of partial differential equations (PDEs). The intensity field is expanded in terms of the spherical harmonics, where $N$ terms are retained for the $P_N$ approximation [1]. The first order approximation, namely the $P_1$ approximation, results in the RTE being transformed to a simple elliptic partial differential equation [1]. This renders easy solution of the resulting equation and is computationally very efficient. This first-order approximation is known to produce fairly accurate results for optically thick media. However, the major drawback of the $P_1$ method is that it is invalid for non-participating media. In other words, one cannot use this method in a scenario where the medium may be participating in some regions and non-participating in some others. The $P_1$ method is also known to yield poor results in cases where the radiation intensity is strongly directionally dependent, as prevalent in scenarios where
emission from boundaries is dominant (i.e., optically thin cold medium bounded by a combination of hot and cold walls). In addition, the convergence of the \( P_1 \) method is poor if the medium is optically thin, a scenario that renders the governing equations stiff. Nonetheless, because of the low computational cost, this method has been implemented in commercial CFD packages such as FLUENT and CFX, and is quite popular.

In recent years, higher order \( P_N \) approximations, in particular, the \( P_3 \) approximation has been used. However, it has been found that for optically thin situations, the accuracy of the \( P_3 \) approximation, although superior to the \( P_1 \) approximation, is unacceptable [7]. Also, the partial differential equations and associated boundary conditions resulting from use of the \( P_3 \) approximation are quite complex [8, 9], and their numerical solution is exponentially more difficult than solution by the \( P_1 \) approximation.

1.2.5 Discrete Ordinates Method (DOM)

The Discrete Ordinates Method (DOM) was originally proposed by Chandrasekar [10] and was applied to astrophysical and atmospheric radiation. Carlson and Lathrop [11, 12] extended its application to the neutron transport field and Fiveland [13, 14], and Truelove [15, 16] developed and implemented the method for all the radiative heat transfer analysis. This method is also available as an option in most commercial CFD packages.
In this method, the entire solid angle $4\pi$ is discretized using a finite number of ordinate directions - $N_{\text{dir}}$, each with its corresponding weight factors. The $N_{\text{dir}}(n = 1..N_{\text{dir}})$ discrete values of direction cosines, $\zeta_n, \eta_n, \mu_n$ satisfy the identity $\zeta_n^2 + \eta_n^2 + \mu_n^2 = 1$. The RTE is written for each ordinate direction and the integral terms are approximated by a numerical quadrature summed over each ordinate direction. This leads to a great dependency of the accuracy on the method on the quadrature scheme used. As a result, one main drawback of this method is that conservation of energy is not always ensured because of the use of quadrature for numerical integration.

Some of the other shortcomings of the Discrete Ordinates Method are the perceived effects such as “false scattering” and “ray effect”. False scattering is caused by the spatial discretization error and results in smearing the intensity distribution and can generally be overcome by using either a finer spatial mesh or a higher order method in space. On the other hand, the so called “ray effect” is a result of errors that arise due to finite discretization of the angular space. It can be reduced by using a finer angular grid, though it cannot be completely eliminated unless an infinite number of directions are used. This ray effect is very prominent in situations where we might have high emission in a very small zone in an enclosure. In such cases, the intensity from this zone will be carried away into the enclosure in the directions of the discrete ordinates. However, as we move away from the zone, these rays may become so far apart that some control volumes or surfaces may not receive any energy from this high-emission zone at all giving rise to unphysical results, as will be demonstrated in this work.
Despite these drawbacks, the popularity of DOM stems from the fact that it has shown promising accuracy over a wide range of optical thicknesses and is readily extendable to higher orders. A number of schemes have been proposed to alleviate this method’s major shortcoming - the ray effect. Amongst them, the most popular one suggested distributing the propagating energy over the entire control angle (pencil of energy) rather than having it propagate along a discrete direction, leading to the finite-volume based Discrete Ordinates Method that is discussed in the following section.

1.2.6 The Finite-Volume Method for Radiation

Over the last couple of decades, the so-called finite-volume method has been accepted and widely used for solution of the conservation equations encountered in fluid flow, primarily because of the exact satisfaction of the conservation equations over the computational domain. Applying the same philosophy to the solution of the RTE, the idea of finite-volume was extended to directional variation in the angular space. This was done by replacing the quadratures in DOM by finite solid angles (control angles) that not only overcomes the problem of energy conservation as discussed above, but also shares the same philosophy of the solution technique and the computational grid as the fluid flow solvers. Essentially, the DOM is analogous to a finite difference method for spatial discretization, while the control angle based DOM is analogous to the finite-volume method. To differentiate this method from the finite-volume method in space, we will refer to it as the Control Angle Discrete Ordinates Method (CADOM) for the remainder of this thesis. The CADOM was
first developed by Raithby and Chui [17] and Hai et al. [18], and was then extended to various problems - Non-orthogonal meshes [19, 20], cylindrical enclosures [21, 22], unstructured meshes [23, 24, 25], periodic geometries [26], and irregular geometries [27].

However, this method also suffers from a few well-known shortcomings. First, the number of partial differential equations that need to be solved in this method is quite large. While low angular resolutions are enough for optically thick scenarios, a much higher angular resolution is necessary for optically thin media in complex 3D geometries. This makes this method computationally very expensive [28]. Secondly, if scattering is present, the task is made more difficult because the directional equations get coupled through the in-scattering term (the last term in Eqn. 1.3), and either iterations or coupled solvers are necessary, both of which add burden to the solution procedure, the former adversely affecting the computational efficiency and the latter requiring more memory and sophisticated solvers.

In iterative solvers, to obtain the intensity in a particular direction, the intensities in all other directions are assumed to be known from the previous iteration, i.e, they are lagged, and appear in the source term on the right hand side of the equation. The newly obtained intensities are then used to update the in-scattering terms, and the process is repeated till convergence. For optically thin media, the angular coupling between the terms are very small and convergence is fast. However, as the optical thickness increases, there is stronger angular coupling and the “lagged” terms become stronger, and convergence is drastically slowed down. This led to the development of
numerous acceleration schemes to improve the convergence and to reduce the solution cost.

Over the years, a number of schemes have been developed to accelerate the convergence of the DOM/CADOM based RTE solvers. An implicit method was proposed by Raithby and Chui [21] to accelerate the CADOM, which was based on multiplicative correction. Fiveland and Jesse [29] studied three acceleration schemes for the RTE including successive over-relaxation, syntax acceleration and mesh rebalance methods. Though the mesh rebalance method was considered the most promising method amongst all the available acceleration schemes, it failed to produce convergence of the RTE for large optical thicknesses and fine grids. This is a major drawback and makes these methods ineffective since refined meshes are essential for obtaining accurate solutions. With the motive of overcoming this problem, Fiveland and Jesse came up with the coarse mesh rebalance (CMR) method [29]. This method is identical to the basic mesh rebalance method except that a coarser mesh is used for the rebalance equation (the implicit equation) for the RTE. In this method, control volumes of the basic mesh are re-grouped into a number of blocks such that each block has a cell optical thickness of around unity. This was shown to give improved performance for simple benchmark problems on uniform grids. However, a general re-grouping algorithm has not yet been proposed and extension of this method to complex geometries and unstructured grids is still under question.

As another remedy, Raithby and Chui [30] showed that the poor convergence of the multiplicative acceleration scheme can be improved by introducing under-relaxation
to damp the interaction between the RTE and the implicit equations of the multiplicative method. However, the choice of the under-relaxation factors are quite arbitrary and are grid dependent.

Another method, namely the Coupled Ordinates Method (COMET), has been developed by Mathur and Murthy [31, 32]. It is based on the multi-grid idea that solves the discrete energy and intensity equations at each cell simultaneously. In this method, at any given node, the intensities in all directions and the temperature are updated together. At each cell in each mesh level, the energy and intensity corrections are solved in a point coupled fashion by inversion of a local matrix, with values at spatial neighbors being known at previous iteration values. However, the complexity of this method increases sharply as the scattering phase function becomes more complicated.

The preceding discussion clearly shows the lack of a single robust, accurate and computationally efficient method for modeling thermal radiation that is accurate over a wide range of optical thicknesses. At the same time, it is clear that different methods have notable advantages for certain scenarios. Therefore, keeping in mind the pros and cons of the established afore-mentioned methods, researchers have started exploring “hybrid” methods.

1.3 Hybrid Methods

Hybrid methods for solving the RTE that employ a variety of different philosophies have been attempted in the past. In almost all cases, the objective has been to
improve the accuracy and/or efficiency of a stand alone RTE solver. A few of the notable popular hybrid methods that have been developed thus far will be discussed in the sections to follow.

1.3.1 Improved Differential Approximation (IDA)

The Improved Differential Approximation (IDA) was first applied by Modest [33], and later, extended to two-dimensional non-scattering media at radiative equilibrium. The differential approximation or the $P_1$ approximation, that yields good results for optically thick regimes, was modified to improve the accuracy in other regimes. The exact integral expression used for computing the intensity due to emission by the medium was approximated by an algebraic expression that combines the optically thick solution with a number of geometrical parameters that became important in optically thin situations. This method has been extended to linear anisotropically scattering three-dimensional media, both in the cases of radiative equilibrium and otherwise, by Modest. However, the major weakness of this method is that, in the case of situations in radiative equilibrium, the method predicts a heat flux that slightly fluctuates around the exact value, and radiative equilibrium is not satisfied exactly.

1.3.2 $Q_L$ Method

This method was developed by Raithby and his co-workers [34, 35]. In this method, an average intensity for each control volume was determined much like the $P_1$ approximation. Hence, a single equation for the intensity in each control volume is derived and the heat flux at the integration points is obtained by re-arranging the
RTE. The radiant energy in a control volume is conserved in all directions but the
directional effects are included in the solutions by a phase weight concept. Recently
[35], it has been extended to include anisotropic scattering as well. Though this
method shows good accuracy and reduced computational cost, it still remains to be
tested for complex 3D geometries and inhomogeneous media.

1.3.3 Modified Differential Approximation

Another hybrid approach that has been proposed is the so-called Modified Differ-
ential Approximation (MDA). Originally proposed by Olfe [36] and later generalized
by Modest [37], the method has been found to be quite accurate over a large range
of optical thicknesses. In this method, the intensity is split into a “wall-emitted”
component, and a “medium-emitted” component. Keeping this philosophy in mind,
researchers have come up with different solution techniques to solve for both the
intensity components.

Proposed by Sakami and Charette [38], the Modified Discrete Ordinates method,
is based on the MDA approximation. The wall-emitted component that is due to
emission and reflection from the walls, represents the residual intensity at any given
location after its attenuation by the absorbing and scattering medium. The medium-
emitted component at the same location is due to emission and in-scattering. The
attenuated wall intensity is evaluated analytically. The enclosure is broken into \( N \)
sub-surfaces of equal intensity and this wall-emitted component is computed by the Zonal
Method, and the radiosities are evaluated numerically through Gaussian quadrature.
The medium component is solved by the Discrete Ordinates Method. This technique
showed improved accuracy. In particular, the “ray effect” was alleviated. However, it showed an increase in computational time compared to standard DOM, which in itself is computationally very expensive, as discussed earlier.

Another implementation of the MDA approximation has been recently carried out for arbitrary 3D geometries by Ravishankar et al. [39]. In this method, the wall-emitted component that is perceived to be strongly directional in nature, is determined using a surface-to-surface exchange formulation that uses geometric view-factors. The medium component, on the other hand, is perceived to be fairly diffuse and isotropic in nature, and is determined using the $P_1$ approximation. In this study, it had been shown that the application of the standard MDA approach to complex 3D geometries with obstructions and inhomogeneous media is prohibitive both from a memory and computational efficiency standpoint. The difficulty in this case stems from the use of a view-factor based approach for solving the wall-emitted component of the radiative intensity. In such an approach, ray tracing is necessary to determine obstructions and optical distances, and this represents a major bottleneck in terms of computational efficiency.

Thus, from the above discussions, it is evident that although the philosophy of splitting the intensity into a strongly directional (wall) and weakly directional (medium) component shows promise from an accuracy standpoint, the procedures suggested by past researchers for determining these two components need revamping.
1.4 Objectives of the current work

The objectives of the current work are as follows:

- To formulate and develop a new robust, computationally efficient hybrid method that has acceptable accuracy over a wide range of optical thicknesses.

- To evaluate this method both from an accuracy and computational efficiency standpoint by applying it to complex 2D and 3D geometries with inhomogeneous media by comparing predicted results against benchmark Monte Carlo results as well as with results predicted by other popular RTE solvers.

- To demonstrate the proposed hybrid method for non-gray media, and compare the computational efficiency of this method with other popular methods used for solving the RTE.

1.5 Outline of the Thesis

The remainder of the thesis is structured as follows. Chapter 2 provides the mathematical details of the different methods used to solve the RTE and presents the formulation of the proposed hybrid method, along with a description for the modifications necessary for non-gray media. Chapter 3 describes the numerical procedure employed to solve the governing equations. In Chapter 4, the results of the different test cases are presented, and the accuracy, efficiency, and robustness of the new hybrid method are examined and discussed. Chapter 5 summarizes the major findings of this work, and concluding remarks and suggestions for future work are provided.
CHAPTER 2

METHODS TO SOLVE THE RADIATIVE TRANSPORT EQUATION (RTE)

The Radiative Transfer Equation (RTE) (Eqn. 1.3) is an integro-differential equation in 7 independent variables, namely, 3 spatial coordinates ($x$, $y$, and $z$), 2 angular coordinates ($\theta$, $\psi$), time ($t$) and wavelength ($\lambda$). For most terrestrial applications, the rate of change of intensity with time is very small compared to the speed of light (radiation), and therefore, the first term in the RTE can be neglected. This implies that for most terrestrial applications, the process of radiation can be thought of as an instantaneous phenomenon. Under this approximation, Eqn. 1.3 reduces to

$$\hat{s} \cdot \nabla I_\lambda = \kappa_\lambda I_{b\lambda} - (\kappa_\lambda + \sigma_{s\lambda}) I_\lambda + \frac{\sigma_{s\lambda}}{4\pi} \int_{4\pi} I_\lambda(\hat{s}_i) \Phi_{s\lambda}(\hat{s}_i, \hat{s}) d\Omega_i$$  \hfill (2.1)

The RTE is not coupled across wavelengths and hence can be solved for each wavelength separately, thus resulting in a 6-dimensional equation. For a general absorbing-emitting-scattering medium, even if the radiative properties are considered spectrally independent or gray, the RTE is still a five-dimensional (3 spatial coordinates and 2 angular coordinates) integro-differential equation and is difficult to solve. As discussed briefly earlier, the directional nature of Eqn. 2.1 makes it difficult to
solve analytically even for simple 1D cases. Hence, approximate solution methods are resorted to. Of the deterministic methods discussed in the previous chapter, since the Discrete Ordinates Method (\(S_N\) Approximation) and the method of Spherical Harmonics (\(P_N\) Approximation) will form the basis for the formulation of the proposed hybrid methodology, these two methods are discussed in further detail in this chapter.

### 2.1 Discrete Ordinates Method (DOM)

The Discrete Ordinates Method (DOM) is based on a discrete representation of the directional variation of the radiative intensity. A solution to the RTE is obtained by solving the transport equation for a set of discrete directions spanning the total solid angle range of \(4\pi\). The standard discrete ordinates method constitutes finite differencing of the directional dependence of the RTE, and the integrals over solid angle are approximated by numerical quadrature, e.g., for the evaluation of the radiative source term, radiative heat flux, etc. Dropping the subscript \(\lambda\) in Eqn. 2.1 for the sake of simplicity of notation, we get

\[
\hat{s} \cdot \nabla I(r, \hat{s}) = \kappa I_b - (\kappa + \sigma_s)I + \frac{\sigma_s}{4\pi} \int_{4\pi} I(r, \hat{s}_i)\Phi_s(\hat{s}_i, \hat{s})d\Omega_i
\]  

(2.2)

In this method, Eqn. 2.2 is solved for a set of \(N_{\text{dir}}\) different directions, \(\hat{s}_i, i = 1,2,\ldots,N_{\text{dir}}\). The angular integration is done by replacing the integrals over direction by numerical quadrature, i.e.,

\[
\int_{4\pi} I(r, \hat{s})d\Omega = \sum_{i=1}^{N_{\text{dir}}} w_i I_i
\]  

(2.3)
where \( w_i \) are the quadrature weights associated with the directions \( \hat{s}_i \). Thus, Eqn. 2.2, an integro-differential equation, under these approximations, leads to \( N_{dir} \) partial differential equations.

\[
\hat{s}_i \cdot \nabla I_i = \kappa I_b - (\kappa + \sigma_s)I_i + \frac{\sigma_s}{4\pi} \sum_{j=1}^{N_{dir}} w_j \Phi_s(\hat{s}_i, \hat{s}_j)I_j
\]

\( \forall i = 1, 2, ..., N_{dir} \)  \hspace{1cm} (2.4)

where \( I_i = I(r, \hat{s}_i) \) has been used for simplicity of notation.

### 2.1.1 Boundary Conditions

In DOM, wherein there are a finite number of discrete directions along which the radiant intensity is tracked, each beam travelling in a direction \( \hat{s}_i \) intersects the enclosure twice, once where the beam emanates from the wall (\( \hat{n} \cdot \hat{s}_i > 0 \)) and once where it strikes the wall, to be absorbed or reflected (\( \hat{n} \cdot \hat{s}_i < 0 \)). The governing equation for the intensity in each direction is first order, requiring only one boundary condition for the emanating intensity (\( \hat{n} \cdot \hat{s}_i > 0 \)). The boundary condition for the above Eqn. 2.4 is given by

\[
I(r_w, \hat{s}_i) = \epsilon(r_w)I_b(r_w) + \frac{\rho(r_w)}{\pi} \sum_{j=1}^{N_{dir}} w_j I(r_w, \hat{s}_j)|\hat{n} \cdot \hat{s}_j|, \quad \text{for} \quad \hat{n} \cdot \hat{s}_i > 0 \hspace{1cm} (2.5)
\]

where \( r_w \) refers to a point on the surface of the enclosure. The set of equations given by Eqn. 2.4, along with their boundary conditions given by Eqn. 2.5, form a set of \( N_{dir} \) simultaneous, first-order linearly coupled partial differential equations for the unknown intensity \( I(r, \hat{s}_i) \). The solution for this intensity in each of the ordinate directions, \( i, I(r, \hat{s}_i) \), can be obtained using an iterative procedure, to be discussed later.
2.1.2 Computation of Incident Radiation and Heat Flux

Once the intensities along the different ordinate directions have been computed, the desired directionally-integrated quantities are easily determined. The incident radiation, $G$, at any location $r$ is determined as follows:

$$G(r) = \int_{4\pi} I(r, \hat{s}) d\Omega \approx \sum_{i=1}^{N_{\text{dir}}} w_i I_i(r) \quad (2.6)$$

The radiative heat flux $q(r)$ inside the medium or at any surface is computed as shown below:

$$q(r) = \int_{4\pi} I(r, \hat{s}) \hat{s} d\Omega \approx \sum_{i=1}^{N_{\text{dir}}} w_i I_i(r) \hat{s}_i \quad (2.7)$$

The surface heat flux can also be found by surface energy balances as

$$q \cdot \hat{n}(r_w) = \epsilon(r_w)[\pi I_b(r_w) - H(r_w)] \quad (2.8)$$

where $H(r_w)$ is the incoming radiation to the surface and is given by

$$H(r_w) \approx \sum_{\hat{n} \cdot \hat{s}_j < 0, j=1}^{N_{\text{dir}}} w_j I_j(r_w)[\hat{n} \cdot \hat{s}_j] \quad (2.9)$$

For engineering calculations, the divergence of heat flux within the computational domain is a quantity of interest. This appears as a sink term in the overall energy conservation equation, Eqn. 1.1, when heat transfer by radiation is included. After determining the incident radiation $G$, we can compute the divergence of heat flux using Eqn. 2.10.

$$\nabla \cdot q = -\kappa (4\pi I_b - G) \quad (2.10)$$
2.1.3 Discrete Ordinate Directions

The choice of the numerical quadrature scheme replacing the directional integrals is arbitrary, although there are some restrictions on the directions $\hat{s}_i$ and the quadrature weights $w_i$ to preserve symmetry. It has been customary to choose sets of directions and weights that are completely symmetric, sets that are invariant after any rotation by $90^\circ$, and satisfying the zeroth, first, and second moments as given below [1].

\[
\int_{4\pi} d\Omega = 4\pi = \sum_{i=1}^{N_{dir}} w_i
\]  
(2.11)

\[
\int_{4\pi} \hat{s} d\Omega = 0 = \sum_{i=1}^{N_{dir}} w_i \hat{s}_i
\]  
(2.12)

\[
\int_{4\pi} \hat{s}\hat{s} d\Omega = \frac{4\pi}{3} \delta = \sum_{i=1}^{N_{dir}} w_i \hat{s}_i \hat{s}_i
\]  
(2.13)

where $\delta$ is the unit tensor.

The number of directions, $N_{dir}$, can be chosen according to the order of the $S_N$ approximation. For the $N^{th}$ order $S_N$ approximation, there are always $N_{dir} = N(N + 2)$ directions to be considered in 3D, while in 2D, the number of directions reduces by a factor of 2. For example, the $S_4$ approximation requires 12 angles (12 partial differential equations) in 2D and 24 angles in 3D. The choice of the order is very important as a higher angular resolution is necessary for optically thin scenarios. This limitation is one of the main drawbacks of the standard DOM as it gives rise to the “ray effect” described earlier. Attempts to alleviate this led to the development
of the Control Angle Discrete Ordinates Method (CADOM) that is based on the finite-volume approach in the angular space, which is discussed next.

2.2 Control Angle Discrete Ordinates Method (CADOM)

The Control Angle Discrete Ordinates Method (CADOM) involves solving the RTE over a discrete number of finite solid angles. The angular space $4\pi$ at any spatial location is discretized into discrete non-overlapping solid angles $\Omega_i$, the centroids of which are denoted by the vector $\mathbf{s}_i$. The finite-volume method uses exact integration to evaluate the solid angle integrals. This method is fully conservative and there is no loss of radiative energy. Though the distribution of angular space can, in principle, be unstructured, a structured discretization is adopted here, with each octant discretized into $N_\theta \times N_\psi$ solid angles. The angles $\theta$ and $\psi$ are the polar and azimuthal angles respectively, and are measured with respect to the global Cartesian system ($X, Y, Z$). $\theta$ is measured from the $Z$ axis and $\psi$ is measured from the $X$ axis (refer to Fig. 2.1).

The angular discretization is uniform in the polar direction and is divided into $N_\theta$ angles. Similarly, there are $N_\psi$ equal angles in the azimuthal direction. However, the subtended solid angles are not equal, and vary with $\theta$. The quantities $\theta_i$ and $\psi_i$ denote the polar and azimuthal angles associated with the centroid of the solid angle $\omega_i$ whose extents are given by $\Delta\theta$ and $\Delta\psi$. The “ray effect” is alleviated in this method since the radiation energy is not assumed to follow a single ray but rather, a pencil of rays.
Angular integration of Eqn. 2.2 results in the following equation.

\[ \mathbf{S}_i \cdot \nabla I(r, \hat{s}_i) = (\kappa(r)I_b(r) - \beta(r)I(r, \hat{s}_i))\Omega_i + \Omega_i \frac{\sigma_s}{4\pi} \sum_{j=1}^{n} \Omega_j \Phi(\hat{s}_i, \hat{s}_j)I(r, \hat{s}_j) \]  

(2.14)

where the integrated direction vector, \( \mathbf{S}_i \), is given by

\[ \mathbf{S}_i = \sin(\phi_i)\sin\left(\frac{\Delta\phi}{2}\right)\Delta\theta\cos(2\theta_i)\sin(\Delta\theta)\mathbf{i} + \cos(\phi_i)\sin\left(\frac{\Delta\phi}{2}\right)\Delta\theta\cos(2\theta_i)\sin(\Delta\theta)\mathbf{j} + \frac{\Delta\theta}{2}\sin(2\theta_i)\sin(\Delta\theta)\mathbf{k} \]  

(2.15)

and the solid angle of integration \( \Omega_i \) is given by

\[ \Omega_i = 2\sin\theta_i\sin\frac{\Delta\theta}{2}\Delta\phi \]  

(2.16)
The above equation in its discrete form becomes

$$\mathbf{S}_i \cdot \nabla I_i = \kappa \Omega_i I_b - (\kappa + \sigma_s) \Omega_i I_i + \frac{\sigma_s}{4\pi} \Omega_i \sum_{j=1}^{N_{dir}} \Omega_j \Phi_s(\hat{s}_j, \hat{s}_i) I_j$$  \hspace{1cm} (2.17)

The boundary conditions for the above equation 2.17 are the same as that for standard DOM in (Eqn. 2.5), with the quadrature weights now being replaced by the solid angles $\Omega_i$. The heat fluxes at the walls can be evaluated in a similar fashion.

### 2.3 Method of Spherical Harmonics ($P_N$)

This method was first proposed by Jeans [40]. Under the $P_N$ approximation, the intensity field, $I$, at a position $\mathbf{r}$ is described as the value of a scalar function on the surface of a sphere of unit radius around the point $\mathbf{r}$. This intensity field can be expressed in terms of a Fourier series as

$$I(\mathbf{r}, \hat{s}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} I_l^m(\mathbf{r}) Y_l^m(\hat{s})$$  \hspace{1cm} (2.18)

where $I_l^m(\mathbf{r})$ are position dependent coefficients and the $Y_l^m(\hat{s})$ are spherical harmonics that are given by

$$Y_l^m(\hat{s}) = (-1)^{\frac{m+|m|}{2}} \left( \frac{(l - |m|)!}{(l + |m|)!} \right)^{\frac{1}{2}} e^{im\psi} P_l^{|m|} \cos \theta$$  \hspace{1cm} (2.19)

that satisfy Laplace’s equation in spherical coordinates. Here, $\theta$ and $\psi$ are the polar and azimuthal angles of the direction unit vector $\hat{s}$, and $P_l^m$ are the associated Legendre polynomials.

The scattering phase function in gray media, $\Phi_s(\hat{s}_i, \hat{s})$, can also be expanded in terms of the Legendre polynomials. For anisotropic scattering, the expansion can be
written as

\[ \Phi_s(\hat{s}_i, \hat{s}) = 1 + \sum_{j=1}^{\infty} A_j P_j(\hat{s}_i, \hat{s}) \] (2.20)

In the \( P_N \) method, integration over all lines of sight (or solid angles) is performed analytically using orthogonal basis functions that are the Legendre polynomials in spherical coordinates, and hence, no angular discretization is necessary.

An approximation is made to the above formulation by considering values of \( l \) only upto \( N \). All the coefficients \( I^m_l(r) \) for \( l > N \) are set to zero. Following this, all the terms containing \( Y^m_l(r) \) are gathered. Since the \( Y^m_l(r) \) are orthogonal to each other, on multiplying and integrating over all directions, \((N + 1)^2\) equations are obtained. Following this, all the coefficients \( I^m_l(r) \) in which \( l \) is odd, are substituted in terms of those with \( l \) being even using a recurrence relation described in [41]. Finally, \((N + 1)^2/4\) partial differential equations are obtained. For example, the lowest order \( P_N \) method, namely the \( P_1 \) method, results in a single Helmholtz equation with Robin-type boundary conditions, that is described in the following section.

### 2.3.1 \( P_1 \) Approximation

The \( P_1 \) approximation to the RTE is obtained by considering Legendre polynomials upto order 1. As a result of this truncation of the series expansion, the incident radiation \( I(r, \hat{s}) \) can expressed as

\[ I(r, \hat{s}) = \frac{1}{4\pi}(G(r) + 3q(r) \cdot \hat{s}) \] (2.21)
where $G(r)$ and $\mathbf{q}(r)$ are the incident radiation and the heat flux vector respectively, that are defined in Eqs. 2.6 and 2.7.

The anisotropic scattering phase function for the $P_1$ approximation is, likewise, approximated by a single term, thereby reducing Eqn. 2.20 to yield

$$
\Phi_s(\hat{s}_i \cdot \hat{s}) = 1 + A_1 \hat{s}_i \cdot \hat{s}
$$

Substitution of Eqns. 2.21 and 2.22 into the RTE (Eqn. 2.1) results in a Helmholtz equation for the incident radiation, $G$, which is of the following form:

$$
\nabla \cdot \left( \frac{1}{(\kappa + \sigma_s - A_1 \sigma_s/3)} \nabla G \right) - 3\kappa G = 4\kappa \pi I_b
$$

Eqn. 2.23 is an elliptic partial differential equation requiring a single boundary condition specified at all boundaries. The following section discusses how the boundary conditions for the $P_1$ approximation are obtained.

## 2.3.2 Boundary Conditions

The boundary condition for the above equation is obtained by minimizing the difference between the intensity predicted by the $P_1$ equations and the actual surface intensities at the walls. Marshak [41] proposed to do this in an integral sense. For an $N^{th}$ order approximation,

$$
\int_{\hat{n} \cdot \hat{s} > 0} I(\mathbf{r}_w, \hat{s}) Y^m_k d\Omega = \int_{\hat{n} \cdot \hat{s} > 0} I_s(\mathbf{r}_w, \hat{s}) Y^m_k d\Omega, \quad -k < m < k, \quad k = 1, 3, \ldots N
$$

where $\mathbf{r}_w$ is the position on the wall and $Y^m_k$ is the associated Legendre polynomial written in a coordinate system local to the boundary. Substituting for the intensity
field, $I$, as given by Eqn. 2.21, followed by tedious algebra, results in a Robin-type boundary condition:

$$-\frac{2 - \epsilon}{\epsilon} \frac{2}{3(\kappa + \sigma_s) - A_1(\sigma_s)} \hat{n} \cdot \nabla G + G = 4\pi I_{bw}$$ (2.25)

where $\hat{n}$ is the surface normal pointing out of the surface, $\epsilon$ is the emissivity of the boundary surface, and $I_{bw}$ is the blackbody radiation intensity at the wall.

### 2.3.3 Heat flux and its divergence

Once the incident radiation has been determined by solution of Eqn. 2.23 along with the boundary conditions given in Eqn. 2.25, the radiative heat flux is found from [1]

$$q = -\frac{1}{3(\kappa + \sigma_s) - A_1} \nabla G$$ (2.26)

and the normal heat flux at a boundary is given by [1]

$$q \cdot \hat{n} = \frac{\epsilon}{1 - \epsilon} (\pi I_{bw} - J_w)$$ (2.27)

where $I_{bw}$ is the blackbody radiative intensity at the boundary and $J_w$ is the radiosity at the boundary. Expressing the radiosity at the boundary in terms of the incident radiation $G$ at the walls, the normal heat flux can also be expressed as [1]

$$q_n = q \cdot \hat{n} = \frac{\epsilon}{2(2 - \epsilon)} (4\pi I_{bw} - G)$$ (2.28)

Similarly, the divergence of the heat flux can be computed from Eqn. 2.10.
As discussed in Chapter 1, both these popular methods, $S_N$ and $P_N$ approximations work well only in certain regimes and have their own shortcomings. In light of the advantages of each method and the respective regimes in which they are accurate, a new hybrid $S_N - P_N$ model is proposed.

2.4 Proposed Hybrid $S_N - P_N$ Method

In this work, a hybrid $S_N - P_N$ method is proposed and developed that employs the philosophy of intensity splitting as in the Modified Differential Approximation (MDA). The directional intensity at a point is treated as a combination of two components:

- One representing the component emanating from the bounding walls attenuated by absorption and out-scattering: the ballistic component, $I_w$.
- Other representing the emission from the medium and in-scattering: the diffusive component, $I_m$.

Therefore, we get

$$I(r, \hat{s}) = I_w(r, \hat{s}) + I_m(r, \hat{s}) \quad (2.29)$$

2.4.1 Drawbacks of standard MDA

In the standard MDA approach, the wall component that is perceived to be strongly directional in nature, is determined using a surface-to-surface exchange formulation that uses geometric view-factors. The medium component, on the other
hand, is perceived to be fairly isotropic and is determined using the $P_1$ approximation. The wall emitted radiative intensity $I_w$ satisfies the following governing equation

$$\frac{dI_w}{ds}(r, \hat{s}) = -I_w(r, \hat{s}) \quad (2.30)$$

leading to an analytical solution for $I_w$ as

$$I_w(r, \hat{s}) = \frac{J_w(r_w)}{\pi} e^{-\tau_h} \quad (2.31)$$

where $J_w(r_w)$ is the radiosity at the wall at the point $r_w$ such that $(r - r_w)$ is along $\hat{s}$. The optical distance of the point $r$ from $r_w$, $\tau_h$, is defined by the expression below.

$$\tau_h = \int_0^h \beta dh' \quad (2.32)$$

The radiosity, $J_w(r_w)$, can be expressed as the sum of emission and reflected irradiation as follows.

$$J_w(r_w) = \epsilon \pi I_{bw}(r_w) + (1 - \epsilon) \int_{\hat{n} \cdot \hat{s} < 0} I_w(r, \hat{s}) |\hat{n} \cdot \hat{s}| d\Omega \quad (2.33)$$

where $\epsilon$ is the emissivity and $\hat{n}$ is the outward pointing unit surface normal to the wall. The integral in Eqn. 2.33 is evaluated by breaking up the enclosure surface into $M$ sub-surfaces of constant radiosity. The radiosity of each of these sub-surfaces is given in terms of the associated view-factors between the sub-surfaces as follows.

$$I_i = \epsilon_i \pi I_{bi} + (1 - \epsilon_i) \sum_{j=1}^M e^{-\tau_{ij}} F_{i-j} \quad (2.34)$$

where $F_{i-j}$ are the geometric diffuse view-factors between the sub-surfaces.

Computation of the view-factors appearing in Eqn. 2.34 is cumbersome and computationally very expensive for complex 3D geometries wherein ray tracing has to be
performed first to determine if two surfaces “see” each other in order to determine obstructions and compute optical distances. Secondly, the view-factor matrix which has a size equal to the number of boundary faces squared has to be stored, and, this requires significant amount of memory. This major bottleneck in the implementation of the original MDA algorithm led to the pursuit of this hybrid $S_N - P_N$ scheme that is the main contribution of this work.

2.4.2 Hybrid $S_N - P_N$ Formulation

In the proposed hybrid scheme, the wall component of the radiative intensity is determined without resorting to a view-factor-based approach. This is accomplished using the discrete ordinates method. As will be evident once the mathematical formulation is presented, the main advantage of this hybrid approach over using the discrete ordinates method for direct solution of the RTE is that the directional equations for the wall component of the intensity, unlike those for the total intensity in standard DOM/CADOM, are no longer coupled. Therefore, huge gains in computational efficiency can be realized since no iterations are necessary because of absence of directional coupling. Since the standard discrete ordinates method is known to suffer from “ray effects” and “false scattering”, the control angle discrete ordinates method was also used as an alternative method for determining the “wall-emitted” component. The “medium” component is solved using the $P_1$ approximation, as done in the standard MDA method.

The governing equation for the wall-emitted component now becomes

$$\mathbf{s}_i \cdot \nabla I_w(r, \mathbf{s}_i) = -\beta(r) I_w(r, \mathbf{s}_i)$$  \hspace{1cm} (2.35)
and the modified $P_1$ equation for the medium component is

$$\nabla \cdot \frac{1}{\beta - A_1 \sigma_s/3} \left( \frac{1}{\beta} (\nabla G_m - A_1 \sigma_s q_w) \right) = -\frac{3}{\beta} \left( \kappa (4\pi I_b - G_m) - \sigma_s G_w \right)$$  (2.36)

where $\beta$ is the extinction coefficient of the medium, defined as $(\beta = \kappa + \sigma_s)$. $A_1$ is the linear coefficient in the scattering phase function and $q_w$ is the radiative heat flux vector due to the wall-emitted component of the intensity. $G_w$ and $G_m$ denote the “wall” and “medium” components of the incident radiation $G$, respectively. In the case of isotropic scattering, $A_1 = 0$ and Eqn. 2.36 reduces to

$$\nabla \cdot \left( \frac{1}{\beta} \nabla G_m \right) = -3\kappa (4\pi I_b - G_m) - 3\sigma_s G_w$$  (2.37)

### 2.4.3 Boundary Conditions

The boundary condition for the governing equation of the “wall emitted” component Eqn. 2.35 under the standard discrete ordinates approximation is as follows

$$I(r_w, \hat{s}_i) = \epsilon(r_w) I_b(r_w) + \frac{\rho(r_w)}{\pi} \sum_{j=1}^{N_{dir}} w_j I(r_w, \hat{s}_j) |\hat{n} \cdot \hat{s}_j|, \text{ for } \hat{n} \cdot \hat{s}_i > 0$$  (2.38)

and the boundary condition for the equation governing the “medium” component Eqn. 2.36 is given by

$$\frac{2(2 - \epsilon)}{\epsilon} \left( \frac{1}{A_1 \sigma_s - 3\beta} \right) (\nabla G_m - A_1 \sigma_s q_w) \cdot \hat{n} + G_m = 0$$  (2.39)

Under the scenario of isotropic scattering, $A_1 = 0$, the above general boundary condition simplifies to

$$\frac{-2(2 - \epsilon)}{3\epsilon} \left( \frac{1}{\beta} \nabla G_m \right) \cdot \hat{n} + G_m = 0$$  (2.40)
It is evident that Eqn. 2.40 is similar to Eqn. 2.25 with the walls being at 0 K, since wall emission is accounted for by the $I_w$ component.

### 2.4.4 Heat flux calculation

The incident radiation due to the wall component is computed from

$$G_w(r) = \int_{4\pi} I_w d\Omega$$

(2.41)

The medium component of $G$, namely, $G_m$, is obtained from the solution of Eqn. 2.36. The total incident radiation at any point $r$ inside the medium is then calculated as the sum of the ballistic component and the medium component of the incident radiation, i.e.,

$$G(r) = G_w(r) + G_m(r)$$

(2.42)

At the boundaries, the wall component of the heat flux is computed in a similar fashion as DOM using Eqn. 2.7. The medium component of the heat flux can be evaluated using the following expression.

$$2 \left( \frac{2}{\epsilon} - 1 \right) q_m \cdot \hat{n} + G_m = 0$$

(2.43)

The total normal heat flux at the boundaries can then be computed as the sum of the two individual components.

$$q \cdot \hat{n} = q_w \cdot \hat{n} + q_m \cdot \hat{n}$$

(2.44)
2.5 Non-Gray Media

The equations presented in the preceding section have been presented for a gray medium, that is, a medium whose radiative properties - absorption coefficient $\kappa$, scattering coefficient $\sigma_s$, phase function $\Phi_s$, as well as emittance of boundary surfaces, $\epsilon$, do not vary across the spectrum. While the assumption of gray surfaces is often a good one over the relatively small relevant part of the spectrum, this is nearly never the case for participating medium, for e.g., molecular gas-particulate mixtures. Although the primary focus of this work is not non-gray (spectral) modeling, a brief overview is included here for the sake of completeness. In real applications, since non-gray radiative properties are prevalent, it is important to demonstrate the proposed RTE solver for non-gray calculations.

Molecular gases below dissociation temperatures absorb and emit over a multitude of very narrow spectral lines, which may overlap and form vibration-rotation bands. This results in an absorption coefficient that oscillates wildly within each band and is zero between the bands. Similarly, the absorption and scattering properties of suspended particles may also vary strongly across the spectrum. However, in the presence of particles of varying sizes, the spectral oscillations tend to be damped out so that the assumption of a gray medium becomes reasonable. The relative importance of these bands depends on the temperature of the medium. Like molecular gases, semi-transparent solids and liquids often display strong absorption bands in the infra-red region. Hence, it is essential that accurate solutions to the equation of transfer be determined by taking into account the spectral variation of radiation properties.
Unfortunately, consideration of spectral variations of radiation properties tends to considerably increase the difficulty of solution of the problem, and makes it much more computationally intense. The complexity and time consumption of non-gray property treatment may be decreased considerably if some simple approximations are made for the spectral dependence of the absorption and/or scattering coefficients.

In this work, the step-wise gray model is used for incorporating the effects of absorption - emission bands in the radiative heat transfer calculations. The non-gray character of the mixture is replaced by an equivalent step-wise gray character. The equivalent gray character is obtained by utilizing the mean beam length [42]. In this model, the absorption coefficient is assumed to attain a finite number of values that remain constant over finite wavenumber regions.

![Box model approximation for molecular gases mixed with particles](image)

Figure 2.2: Box model approximation for molecular gases mixed with particles [42]
Figure 2.2 shows a typical spectral variation of the absorption coefficient of a molecular gas accompanied by absorbing and/or scattering particles. For a molecular gas with \( N \) bands, the so-called box model \([42]\) is used to approximate the absorption coefficient as

\[
\kappa_\eta \approx \sum_{l=1}^{N} \kappa_l \left[ H(\eta - \eta_{ol} + \frac{1}{2} \Delta \eta_{el}) - H(\eta - \eta_{ol} - \frac{1}{2} \Delta \eta_{el}) \right]
\]  

(2.45)

where the wavenumber \( \eta \) is the spectral variable, \( \eta_{ol} \) is the wavenumber at the band center, \( \Delta \eta_{el} \) is the equivalent band width and \( \kappa_l \) is the absorption coefficient of the \( l^{th} \) band. The Heaviside’s unit step function is given by

\[
H(x) = 0 \quad \text{if} \quad x < 0
\]

\[
= 1 \quad \text{if} \quad x > 0
\]

To account for absorption and/or scattering by the background particles that can be approximated as gray, a background absorption coefficient \( \kappa_{bg} \) is defined. The total absorption coefficient of the medium can now be expressed as

\[
\kappa_\eta \approx \kappa_{bg} + \sum_{l=1}^{N} \kappa_l \left[ H(\eta - \eta_{ol} + \frac{1}{2} \Delta \eta_{el}) - H(\eta - \eta_{ol} - \frac{1}{2} \Delta \eta_{el}) \right]
\]  

(2.46)

Here, the spectrum has been broken up into \( N \) gray gas bands, and each band \( l \) is modeled as a box with a uniform absorption coefficient \( \kappa_l \) and an equivalent band-width \( \Delta \eta_{el} \).

### 2.5.1 Extension of RTE to Non-Gray Media

Referring to the general RTE for gray media, Eqn. 2.1, a piece-wise integration of this equation is done over different wavelength bands over which the spectral
properties are defined.

\[
\mathbf{s} \cdot \nabla I_{\lambda} d\lambda = \int_{\lambda_1}^{\lambda_2} \kappa_{\lambda}(I_{b\lambda} - I_{\lambda}) d\lambda - \int_{\lambda_1}^{\lambda_2} \sigma_{s\lambda} I_{\lambda} d\lambda + \int_{\lambda_1}^{\lambda_2} \frac{\sigma_{s\lambda}}{4\pi} \int_{4\pi} I_{\lambda}(\mathbf{s}_i) \Phi_{s\lambda}(\mathbf{s}_i, \mathbf{s}) d\Omega_i d\lambda
\]

(2.47)

The emission term, \(\kappa_{\lambda} I_{b\lambda}\), on integration over a given wavelength interval, from \(\lambda_1\) to \(\lambda_2\) gives \(\kappa_{\lambda}\) multiplied by the fraction of blackbody emission between the two wavelengths \(\lambda_1\) and \(\lambda_2\) at the temperature \(T\).

\[
\kappa_{\lambda} \int_{\lambda_1}^{\lambda_2} I_{b\lambda} d\lambda = \kappa_{\lambda} [f(\lambda_2, T) - f(\lambda_1, T)] \frac{\sigma T^4}{\pi}
\]

(2.48)

where \(f\) is the so-called fraction of blackbody radiation. The total intensity, \(I\), over the entire spectrum is computed as follows,

\[
I = \int_{0}^{\infty} I_{\lambda} d\lambda \approx \sum_{l=1}^{N_{\text{bands}}} I_l
\]

(2.49)

where \(I_l\) is defined as follows.

\[
I_l = \int_{\lambda_1}^{\lambda_2} I d\lambda
\]

(2.50)

The RTE is now solved for each band, and the incident radiation, \(G\), obtained from the solution of RTE in each band is summed and the total intensity and heat fluxes are obtained, i.e.,

\[
G = \int_{0}^{\infty} G_{\lambda} d\lambda \approx \sum_{l=1}^{N_{\text{bands}}} G_l
\]

(2.51)

The total heat flux is computed as an integral over the entire spectrum.

\[
q = \int_{0}^{\infty} q_{\lambda} d\lambda \approx \sum_{l=1}^{N_{\text{bands}}} q_l
\]

(2.52)
In this chapter, the governing equations for the three different methods that will be explored in this work, namely, the discrete ordinates method, method of spherical harmonics, and the new hybrid $S_N - P_N$ method, were presented. The extension of the RTE for non-gray media was also briefly described. The next chapter will discuss the numerical formulation and solution technique employed for obtaining a solution to these governing equations.
CHAPTER 3

NUMERICAL PROCEDURE

In the preceding chapters, the governing equations for the Discrete Ordinates Method (DOM and CADOM), $P_1$ approximation, and the hybrid $S_N - P_N$ method were presented. In this chapter, the numerical methods used to obtain the solution to these governing equations will be described.

The governing equations for standard DOM, CADOM, $P_1$, and the hybrid $S_N - P_N$ methods are discretized using the unstructured finite-volume procedure. While DOM and CADOM solve the RTE by conserving radiant energy in each discrete direction for each control volume, the $P_1$ approximation has been formulated to conserve energy in all directions in each control volume. The procedure adopted to convert the governing differential equations for each of these methods to a set of linear algebraic equations is discussed in the following section.

3.1 Discrete Ordinates Method

The RTE, under the standard discrete ordinates approximation, in its divergence form, may be written as
\[ \nabla \cdot (I_i \hat{s}_i) = \kappa I_b - (\kappa + \sigma_s) I_i + \frac{\sigma_s}{4\pi} \sum_{j=1}^{N_{dir}} w_j I_j \Phi_{ij}, \quad \forall i = 1, 2...N_{dir} \quad (3.1) \]

where \( w_j \) is the weight factor for the direction \( \hat{s}_j \). Performing an integration over a finite-volume, followed by application of the Gauss-divergence theorem yields

\[ \int_{V_o} \nabla \cdot (I_i \hat{s}_i) dV = \int_S I_i \hat{s}_i \cdot \hat{n} dA = \kappa_o V_o I_{bo} - \beta V_i I_{io} + \frac{\sigma_s V_o}{4\pi} \sum_{j=1}^{N_{dir}} w_j \Phi_{ij} I_{jo} \quad (3.2) \]

where the subscript “o” represents the value at the cell \( O \) and \( V_o \) denotes the volume of the control volume.

\[ \begin{align*}
\text{\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{3d_volume_element}
\caption{Schematic of Unstructured 3D Volume Element}
\end{figure}}
\end{align*} \]

In the case that the control volume is a convex polyhedron bounded by discrete faces, as in the case of an unstructured mesh, shown in Fig. 3.1, the surface integral in Eqn. 3.2 may be replaced by a discrete summation over all faces of the polyhedron, yielding
\[ \sum_f (\hat{s}_i \cdot \hat{n}_f) A_f I_{i,f} = \kappa_o V_o I_{b,o} - \beta_o V_o I_{i,o} + \frac{\sigma_{so} V_o}{4\pi} \sum_{j=1}^{N_{dir}} w_j \Phi_{ij} I_{j,o} \quad \forall i = 1, 2, ..N_{dir} \] (3.3)

where the direction vector \( \hat{s}_i \) is given by

\[ \hat{s}_i = \sin\theta \sin\phi \hat{i} + \sin\theta \cos\phi \hat{j} + \cos\theta \hat{k} \] (3.4)

and \( \hat{n}_f \) is the outward pointing surface normal of the faces of the control volume. \( A_f \) is the area of the face \( f \), and \( V_o \) is the volume of the control volume. In the above discretized form of the DOM equation, it should be noted that there appears a term involving the face intensities - \( I_{i,f} \). A number of schemes have been proposed for the treatment of the face intensities [1]. Here, a first order upwind scheme has been adopted.

\[ I_{i,f} = I_{i,o} \quad \text{if} \quad \hat{s}_i \cdot \hat{n}_f > 0 \]
\[ = I_{i,N} \quad \text{if} \quad \hat{s}_i \cdot \hat{n}_f < 0 \] (3.5)

where \( N \) denotes the neighbor to cell \( O \), as shown in Fig. 3.1. It is this first-order approximation that usually causes the so-called “false scattering”. Nevertheless, since higher-order schemes are considerably more computationally expensive and tedious to implement, and because the problem can be alleviated by using a fine mesh, we choose to use a first-order upwind scheme. With this treatment for the face intensities, upon rearranging Eqn. 3.3, the following equation is obtained.

\[ (\beta_o V_o - \frac{\sigma_{so}}{4\pi} w_i \Phi_{ni} V_o + C_o) I_{i,o} - \sum_N D_{oN} I_{i,N} = \kappa_o V_o I_{b,o} + \frac{\sigma_{so} V_o}{4\pi} \sum_{j=1,j\neq i}^{N_{dir}} w_j \Phi_{ij} I_{j,o}, \]
\[ \forall i = 1, 2, ...N_{dir} \] (3.6)
where \( C_o = \sum_N (\hat{s}_i \cdot \hat{n}_f) A_f \) and \( D_{oN} = \text{Max}(0, -\hat{s}_i \cdot \hat{n}_f) A_f \). In the above equation, \( I_{io} \) and \( I_{iN} \) denote the intensity in direction \( i \) in cell \( O \) and the neighboring cell \( N \), respectively. Eqn. 3.6 represents a set of \( N_{\text{dir}} \) algebraic equations for the intensities in each direction in each cell in the domain. However, these set of equations become coupled due to the presence of the in-scattering term, (the last term of Eqn. 3.6), involving intensities in other directions. Hence, obtaining a direct solution for the intensities in all the directions becomes difficult, especially in optically thick scattering media when the equations become strongly coupled. Hence, an iterative solution procedure is adopted. The contribution to the in-scattering term from other directions is treated explicitly, i.e., it is computed from previous iteration values, and is added to the source term \( \kappa_b I_{bo} \). The resulting algebraic equations are solved using the Generalized Minimum Residual (GMRES) solver after incomplete LU (ILU) pre-conditioning.

### 3.2 Control Angle Discrete Ordinates Method

The governing equations for CADOM are discretized in a similar fashion as done for standard DOM. The resulting discretized equations are

\[
\sum_f (\mathbf{S}_i \cdot \hat{n}_f) A_f I_{if} = \kappa_o \Omega_i V_o I_{bo} - \beta_o \Omega_i V_o I_{io} + \frac{\sigma_{so} \Omega_i V_o}{4\pi} \sum_{j=1}^{N_{\text{dir}}} \Omega_j \Phi_{ij} I_{jo} \quad \forall i = 1, 2, \ldots N_{\text{dir}}
\]  

(3.7)

where here \( \Omega_i \) represents the solid angle and the integrated direction vector \( \mathbf{S}_i \) is as defined in Eqn. 2.15. The same treatment for face intensities is used as in DOM, and the resulting algebraic equations are solved iteratively in the same manner.
3.3 \(P_1\) Approximation

In contrast to DOM and CADOM, where intensities along each direction and in each cell are solved for, in the \(P_1\) approximation, the total incident radiation \(G\) (integrated intensity in over all directions) at each cell is computed directly.

Referring to Eqn. 2.23, the governing equation for the \(P_1\) approximation and Eqn. 2.25, the boundary condition, and performing a finite-volume integration, followed by application of the Gauss divergence theorem yields,

\[
\sum_f \left( \frac{1}{(3\beta_f - A_1\sigma_{s,f})} \hat{n}_f \cdot \nabla G_f \right) A_f = -\kappa_o (4\pi I_{bo} - G_o)V_o \tag{3.8}
\]

In this case, it is necessary to express the normal diffusive flux at each face in terms of the cell-center values prior to solution of Eqn. 3.8. After some tedious algebra, it can be shown that

\[
\hat{n}_f \cdot \nabla G_f = \frac{G_N - G_o}{\delta_f} - \frac{[\hat{n}_f \times \nabla G_f] \times \hat{n}_f}{\delta_f} \frac{l_f}{\delta_f} = \frac{G_N - G_o}{\delta_f} - \frac{J_{T,f}}{\delta_f} \tag{3.9}
\]

where \(\delta_f = \hat{n}_f \cdot l_f\) is the distance in the direction of the surface normal between the two cells straddling the face \(f\) (Fig. 3.1). Essentially, in the above derivation, the flux normal to a cell face has been decomposed into a flux along the vector joining the two cell centers straddling the face and a flux tangential to the face, \(J_T\). In our treatment, the first term of the right hand side of Eqn. 3.9 is treated implicitly, while the second term is treated explicitly. The computation of the second term requires determination of vertex values and further application of the divergence theorem. The derivation of the exact expression for this term is rather lengthy and is omitted here.
for the sake of brevity. For boundary faces, the normal flux, \((\hat{n}_f \cdot \nabla G_f)\), is replaced by the boundary condition as given in Eqn. 2.25. The final discretized equations are as follows.

\[
\left(\sum_f \frac{A_f}{\delta_f (3\beta_f - A_1\sigma_{s,f})} + \kappa_o V_o\right) G_o - \sum_f G_{nb} \frac{A_f}{\delta_f (3\beta_f - A_1\sigma_{s,f})} = -\sum_f \frac{A_f}{\delta_f (3\beta_f - A_1\sigma_{s,f})} J_{T,f} + 4\pi \kappa_o I_b V_o \quad (3.10)
\]

\[
\left(1 + \frac{2(2 - \epsilon)}{\delta_f \epsilon (3\beta_f - A_1\sigma_{s,f})}\right) G_b - \frac{2(2 - \epsilon)}{\delta_f \epsilon (3\beta_f - A_1\sigma_{s,f})} G_o = 4\pi I_{bw} - \gamma_f J_{T,f} \quad (3.11)
\]

where \(\gamma_f\) is defined as

\[
\gamma_f = \frac{2(2 - \epsilon)}{\delta_f \epsilon (3\beta_f - A_1\sigma_{s,f})} \quad (3.12)
\]

and \(G_{nb}\) is the value of \(G\) in the neighboring cell. In these equations, \(G_b\) represents the incident radiation on the boundary face. These set of algebraic equations are also solved iteratively using the preconditioned GMRES solver.

### 3.4 Hybrid \(S_N - P_N\) Method

The numerical treatment of the governing equations for Discrete Ordinates Method and the \(P_1\) approximation were discussed in the previous sections. The discretization of the hybrid \(S_N - P_N\) method will now be presented.

#### 3.4.1 Wall emitted component

If the intensity of the wall-emitted component in the direction is denoted by \(I_{w,i}\), then the governing equation for the wall-emitted component given by Eqn. 2.30 can
be re-written as

$$\nabla \cdot (I_{w,i} \hat{s}_i) = -\beta I_{w,i} \quad (3.13)$$

where $N_{\text{dir}}$ is the total number of discrete angular directions. Eqn. 3.13 represents a set 3-dimensional partial differential equations for all the $N_{\text{dir}}$ directions. Applying the Gauss-divergence theorem, followed by application of a finite-volume integration, the following set of discrete equations are obtained.

$$\sum_f (\hat{s}_i \cdot \hat{n}_f) A_f I_{w,i,f} = -\beta_o V_o I_{w,i,o} \quad (3.14)$$

It can be observed that there is no directional coupling here as the in-scattering terms are now absorbed into the medium component equation. Comparing this equation with Eqn. 3.3, it can be seen that the resulting set of discrete equations obtained here are decoupled from each other and can be solved directly, thus making it much more computationally efficient.

### 3.4.2 Medium component

Referring to Eqns. 2.36 and 2.39, the governing equations and the boundary conditions for the hybrid $S_N - P_N$ method, and following a procedure similar to the $P_1$ approximation, the final discretized equations for $G$ at the cell centers and at the boundaries are obtained.

$$\left(\sum_f \frac{A_f}{\delta_f(3\beta_f - A_1\sigma_{s,f})} + \kappa_o V_o \right) G_{m,o} - \sum_f G_{m,\text{nb}} \frac{A_f}{\delta_f(3\beta_f - A_1\sigma_{s,f})} A_f = -\sum_f \frac{A_f}{\delta_f(3\beta_f - A_1\sigma_{s,f})} J_{T,f} + 4\pi I_b \kappa_o V_o + \sigma_{s,o} G_{w,o} V_o \quad (3.15)$$
\[
\left(1 + \frac{2(2 - \epsilon)}{\delta_f \epsilon (3\beta_f - A_1 \sigma_{s,f})}\right) G_{m,b} - \frac{2(2 - \epsilon)}{\delta_f \epsilon (3\beta_f - A_1 \sigma_{s,f})} G_{m,o} = -\gamma_f J_{T,f} \quad (3.16)
\]

In the above equations, \(G_{m,o}, G_{m,nb}, G_{m,b}\) denote the values of the medium component of the incident radiation at the cell centers, neighboring cells, and at the boundaries respectively. Comparing Eqns. 3.10 and 3.15, it can be seen that the only difference between the two equations is the presence of a "source" term, the last term in Eqn. 3.15, in the latter expression for the hybrid method. This source term is computed from the solution of the wall-emitted intensity equation. Similarly, the boundary conditions for the hybrid method also get modified because the "wall-emitted" component is now accounted for in the ballistic equation.

### 3.5 Solution Algorithm

In order to solve the RTE using the proposed hybrid \(S_N - P_N\) method, the discretized equations discussed in the preceding section must be solved in a certain sequence. The overall algorithm and the critical steps in the algorithm are as follows:

- Solve Eqn. 3.14 using standard DOM or CADOM to determine the wall-emitted component of radiation intensity, \(I_w(r, \hat{s})\).

- Compute the wall-emitted component of the incident radiation, \(G_w\), at all control volumes (cell centers) using \(G_w = \int_{4\pi} I_w d\Omega\) using either the weights in DOM or finite solid angle integration in CADOM. This quantity appears as a source in the governing equation for the medium-emitted component.
• Compute the medium emitted component of the incident radiation, $G_m$, by solving Eqn. 3.15 along with the boundary conditions given by Eqn. 3.16 using an iterative solution procedure.

• Compute the total incident radiation, $G$, using Eqn. 2.42.

• Compute the divergence of heat flux (source term in overall energy equation) using $\nabla \cdot \mathbf{q}_{\text{rad}} = \kappa (4\pi I_b - G)$.

Figure 3.2: Flowchart of solution algorithms for DOM, hybrid $S_N - P_N$ and $P_1$ methods.
As can be seen from the above flowchart in Fig. 3.2, and from the outline of the solution algorithm, the two most critical and time-consuming steps are the determination of the wall-emitted component of the intensity and the medium-emitted component of the intensity. To verify the accuracy and robustness, and to measure the efficiency of the hybrid $S_N - P_N$ method, several 2D and 3D problems have been solved and the results are shown in the next chapter.
CHAPTER 4

RESULTS AND DISCUSSION

In this section, the accuracy and efficiency of the hybrid RTE solver is discussed. A number of test cases have been considered to study the robustness of the hybrid $S_N - P_N$ method. In order to assess the accuracy of the hybrid RTE solver for arbitrary geometry with obstructions, a Monte Carlo code was used to generate benchmark results for isotropically scattering media for arbitrary 2D and 3D geometries. For the test cases in which absorption and emission are considered, Monte Carlo simulation results were not available, and therefore, the results of the new hybrid method are compared with the results of other popular methods. In the final test case, the medium is treated as non-gray and a wide-band model is used. Since this test case is the most complex of the four cases considered, it is also used for computational efficiency studies.

4.1 2D Geometries

In this section, the results generated using DOM, CADOM, $P_1$, and the hybrid $S_N - P_N$ methods are compared against the benchmark Monte Carlo results for a
number of test cases with 2D geometries. Refering to Eqn. 2.32, the optical thickness \( \tau_h \), is first defined. This quantity serves as a parameter for the simulations to be conducted.

\[
\tau_h = \int_0^h \beta \, dh'
\]  

(4.1)

An additional quantity, the scattering albedo \( \omega \), is defined. It gives a measure of the relative importance of scattering in the medium over absorption by the medium.

\[
\omega = \frac{\sigma_s}{\kappa + \sigma_s} = \frac{\sigma_s}{\beta}
\]  

(4.2)

Test Case 1

For the first test case, a 2D square box of size \( h \) was considered. The central 20% of the bottom wall was heated to \( T_h = 1000 \) K and all the other walls are assumed to be at \( T_c = 0 \) K, as shown in Fig. 4.1. All walls are assumed to be black. The optical thickness is varied by three orders by changing the value of \( \beta \) yielding three different values of \( \tau_h = 0.1, 1.0, \) and 10.0. This problem consisted of a gray isotropically scattering medium. The absorption coefficient of the gas was assumed to be zero, implying that \( \beta = \sigma_s \) and \( \omega = 1.0 \). This implies that the enclosure is in radiative equilibrium with just pure redistribution of energy due to scattering within the medium, with no emission or absorption by the medium. The \( S_8 \) approximation (40 angles) was used for standard DOM and 40 angles were used for discretizing the angular space in CADOM.

The non-dimensional heat fluxes along different walls of the square enclosure were computed and compared with the benchmark results. A comparison of the results
obtained by a number of popular RTE solvers, namely - $P_1$, standard MDA, standard DOM, CADOM and the hybrid $S_N - P_N$ method based on standard DOM and CADOM (denoted as DOM-$P_1$ and CADOM-$P_1$, respectively) is presented below.

<table>
<thead>
<tr>
<th>Legend</th>
<th>Explanation of Method used</th>
</tr>
</thead>
<tbody>
<tr>
<td>MDA</td>
<td>Modified Differential Approximation</td>
</tr>
<tr>
<td>Monte-Carlo</td>
<td>Monte Carlo results computed with 10 ensembles.</td>
</tr>
<tr>
<td>$P_1$</td>
<td>Standard $P_1$ Approximation</td>
</tr>
<tr>
<td>DOM</td>
<td>Discrete Ordinates Method</td>
</tr>
<tr>
<td>CADOM</td>
<td>Control Angle Discrete Ordinates Method</td>
</tr>
<tr>
<td>DOM - $P_1$</td>
<td>Hybrid DOM - $P_1$</td>
</tr>
<tr>
<td>CADOM - $P_1$</td>
<td>Hybrid CADOM - $P_1$</td>
</tr>
</tbody>
</table>

Table 4.1: Explanation of legend used in all figures

The results obtained for this test case provide some interesting insights. In the optically thin regime ($\tau_h = 0.1$), from figures 4.2 and 4.3, it can be seen that the DOM
Figure 4.2: Test Case 1 - Non dimensional heat flux along right and top walls for $\tau_h = 0.1$

Figure 4.3: Test Case 1 - Non-dimensional heat flux along bottom wall for $\tau_h = 0.1$
Figure 4.4: Test Case 1 - Non-dimensional heat flux along right and top walls for $\tau_h = 1.0$

Figure 4.5: Test Case 1 - Non-dimensional heat flux along bottom wall for $\tau_h = 1.0$
Figure 4.6: Test Case 1 - Non-dimensional heat flux along right and top walls for $\tau_h = 10.0$

Figure 4.7: Test Case 1 - Non-dimensional heat flux along bottom wall for $\tau_h = 10.0$
solution depicts the expected “ray effect”. The distinct oscillations seen in the heat flux profile predicted by DOM and even the hybrid $S_N - P_N$ based on standard DOM on the top and right wall are a manifestation of the ray effect. This is because of the finite differencing in the angular space using a limited number of angular nodes. With CADOM and subsequently with the hybrid CADOM-$P_1$ solver, this effect is seen to be alleviated to a great extent thus resulting in much better agreement with the Monte Carlo results. As the optical thickness of the media increases, the strong directionality of radiation propagation reduces and both the standard DOM and the hybrid $S_N - P_N$ method based on standard DOM show reduced “ray effect” and their results are closer to the Monte Carlo predictions. It should be noted that though both the hybrid $S_N - P_N$ method and the standard MDA approximation employ the same philosophy of radiative intensity splitting, the standard MDA method does not exhibit the “ray effect” as the wall-emitted intensity is evaluated through an exact viewfactor-based formulation, while in the hybrid $S_N - P_N$ method, the “ray effect” is perceived because of the $S_N$ approximation used for evaluation of the wall intensity. The standard MDA approximation is seen to predict accurately in both the optically thin and thick media but shows deviation in the intermediate regime. It can also be seen that the $P_1$ approximation predicts poorly in optically thin media as it gives unphysical results with the normalized heat flux values exceeding 1.0 at certain locations in the bottom wall for the case with $\tau_h = 0.1$. Even for intermediate optical thickness as can been from figures 4.4 and 4.5, the $P_1$ approximation shows an over prediction when compared to the benchmark Monte Carlo (MC) results along the bottom and right walls. The results from all the methods for the optically thicker regime, shown in figures 4.6 and 4.7, compare well against the Monte Carlo results.
Test Case 2

The next test case considered was that of a solid 2D opaque box inside a larger 2D box with radiation transport in the gap between the two boxes as shown in Fig. 4.8(a) - a case that was specifically designed to study the effect of obstructions in the geometry. All walls were assumed to be black and the absorption coefficient of the gas, $\kappa$, was assumed to be zero. A gray isotropically scattering medium was considered. Three different values of optical thickness, based on the size of the larger box, were considered for the present study, namely $\tau_h = 0.1, 1$ and 10.

These results were computed with 7500 triangular cells, and the computational mesh is shown in Fig. 4.8(b). The benchmark Monte Carlo results were generated with 2.72 million rays and 10 ensembles were considered for statistical averaging.

Figures 4.9, 4.10, 4.11, and 4.12 show the non-dimensional radiative heat fluxes (normalized by $\sigma T_h^4$) predicted by the various methods for $\tau_h = 0.1$. The results shown in these figures highlight several important findings. First, on similar lines as the previous test case, the standalone $P_1$ approximation produces physically meaningless results as indicated by non-dimensional heat fluxes exceeding unity. The solutions produced by either the standard discrete ordinates method (DOM) or the DOM-based hybrid method (DOM-$P_1$) exhibit strong oscillations, a manifestation of the well-known ray effects. Both CADOM as well as the hybrid CADOM-$P_1$ method appear to produce very accurate results. The CADOM results and the hybrid CADOM-$P_1$ results agree well with the standard MDA method, and are found to be almost identical to each other. This is to be expected for this optically thin case, in which the overall solution of the hybrid method is dominated by the wall-emitted component.
Figure 4.8: 2D Box in Box geometry

(a) Box in Box with obstructions

(b) Mesh used - 7420 cells
Figure 4.9: Test Case 2 - Non-dimensional heat flux along top wall for $\tau_h = 0.1$

Figure 4.10: Test Case 2 - Non-dimensional heat flux along bottom wall for $\tau_h = 0.1$
Figure 4.11: Test Case 2 - Non-dimensional heat flux along inner top wall for $\tau_h = 0.1$

Figure 4.12: Test Case 2 - Non-dimensional heat flux along inner bottom wall for $\tau_h = 0.1$
Figure 4.13: Test Case 2 - Non-dimensional heat flux along top wall for $\tau_h = 1.0$

Figure 4.14: Test Case 2 - Non-dimensional heat flux along bottom wall for $\tau_h = 1.0$
Figure 4.15: Test Case 2 - Non-dimensional heat flux along inner top wall for $\tau_h = 1.0$

Figure 4.16: Test Case 2 - Non-dimensional heat flux along inner bottom wall for $\tau_h = 1.0$
The non-dimensional radiative heat fluxes (normalized by $\sigma T^4$) predicted by the various methods for $\tau_h = 1$ are shown in figures 4.13, 4.14, 4.15 and 4.16. In this case, the results obtained using the standard $P_1$ approximation are not as error-prone as for the optically thin case. However, the standard $P_1$ approximation is still the least accurate of all the methods considered. DOM and hybrid DOM-$P_1$ still exhibit ray effects, although the effects are less pronounced than for the optically thin case. The hybrid DOM-$P_1$ method appears to be slightly more accurate than the standard DOM. The standard CADOM as well as the hybrid CADOM-$P_1$ method still exhibit the best accuracy, although these two methods now yield slightly different results because the solution of the hybrid method is now influenced by both the wall-emitted as well as the medium-emitted components.

Figure 4.17: Test Case 2 - Non-dimensional heat flux along top wall for $\tau_h = 10.0$
Figure 4.18: Test Case 2 - Non-dimensional heat flux along bottom wall for $\tau_h = 10.0$

Figure 4.19: Test Case 2 - Non-dimensional heat flux along inner top wall for $\tau_h = 10.0$
A final set of calculations were performed for the same test case with an optically thick medium, i.e., $\tau_h = 10.0$, and these results are shown in Fig. 4.17, 4.18, 4.19 and 4.20. It can be seen that the hybrid results match well with the Monte Carlo results due to dominance of the medium component that is predicted well by the $P_1$ approximation in optically thicker regimes.

4.2 3D geometries

This section presents the results from the numerical implementation of the hybrid $S_N - P_N$ model in 3D geometries. Based upon the observations made from the 2D test cases that CADOM alleviates the ray effect, only the CADOM was pursued for
solution in 3D geometries, both for direct solution of the RTE as well as for solving the “wall-emitted” component in the hybrid method.

Test Case 3

The first 3D geometry used for assessing the accuracy of the proposed method is comprised of a 3D opaque cube contained within a larger 3D cube, i.e., a 3D version of Test Case 2, as shown in Fig. 4.21 (a). The outer enclosure is a cube of side $h$ and the inner enclosure is a cube of side $0.2h$. The distances are non-dimensionalized with respect to the size of the outer enclosure $h$, and so are all the length dimensions in every figure in this section. The mesh used has 55000 tetrahedral cells and is shown in Fig. 4.21 (b).

The walls of the outer enclosure at planes $x = 1$, $y = 0$ and $z = 0$ and the walls of the inner enclosure at $x = 0.4$, $y = 0.6$ and $z = 0.6$ are kept at $T_h = 1000$ K. The other walls are at $T_c = 0$ K. All walls are black. The heat fluxes and differences in heat fluxes shown in this section are non-dimensionalized with respect to $\sigma T_h^4$. The medium is purely scattering as before, and results are compared for three different optical thicknesses $\tau_h = 0.1$, 1.0, and 10.0, that is defined based on the length of a side of the outer enclosure.

Results from four different methods, namely Monte Carlo serving as benchmark, $P_1$ approximation, CADOM and the hybrid $S_N - P_N$ method are presented here. The benchmark Monte Carlo results in this case were generated using 184 million rays and 10 ensembles were considered for statistical averaging.
A grid independence study for this “box in box” geometry was first performed with 55K, 111K, and 260K cells in an unstructured tetrahedral mesh. Since the inner walls represent the coarsest resolution for any given mesh size, the non-dimensional heat flux contours were plotted for the inner cold wall. The non-dimensional heat flux along the diagonal of the inner cold wall was plotted and compared for the three mesh sizes in Fig. 4.22. It was found that grid-independence was achieved at 55K tets for both the CADOM and Hybrid methods. Hence, the 55K unstructured volumetric mesh was used for further studies. An angular grid independence study was subsequently conducted with the 55K unstructured mesh, and it was found that for both CADOM and the hybrid $S_N - P_N$, an angular resolution of 20 X 20 produced results within 1% of an angular resolution of 40 X 40, and was, therefore, deemed appropriate for all future studies in 3D.
The non-dimensionalized radiative heat flux contours plotted along a cold and hot wall of the outer and inner cube are presented here. The errors obtained by comparing the results of CADOM and the hybrid method with the Monte Carlo solutions are also shown below.

Figure 4.22: Test Case 3 - Grid Independence for hybrid $S_N - P_N$
Figure 4.23: Test Case 3, Heat flux contours on hot outer bottom wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$

Figure 4.24: Test Case 3, Heat flux contours on hot outer bottom wall - Monte Carlo and $P_1$ for $\tau_h = 0.1$
Figure 4.25: Test Case 3, Heat flux contours on cold outer back wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$.

Figure 4.26: Test Case 3, Heat flux contours on cold outer back wall - Monte Carlo and $P_1$ for $\tau_h = 0.1$. 70
Figure 4.27: Test Case 3, Percent errors with Monte Carlo for hot outer bottom wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$

Figure 4.28: Test Case 3, Percent errors with Monte Carlo for cold outer back wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$
Figure 4.29: Test Case 3, Heat flux contours on hot inner top wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$

Figure 4.30: Test Case 3, Heat flux contours on hot inner top wall - Monte Carlo and $P_1$ for $\tau_h = 0.1$
Figure 4.31: Test Case 3, Heat flux contours on cold inner front wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$

Figure 4.32: Test Case 3, Heat flux contours on cold inner front wall - Monte Carlo and $P_1$ for $\tau_h = 0.1$
Figure 4.33: Test Case 3, Percent errors with Monte Carlo for hot inner top wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$

Figure 4.34: Test Case 3, Percent errors with Monte Carlo for cold inner front wall - CADOM and $S_N - P_N$ for $\tau_h = 0.1$
Figures 4.23, 4.24, 4.25, and 4.26 show the heat flux contours on the outer bottom (hot) and back (cold) wall computed using 4 different methods - CADOM, hybrid $S_N - P_N$, Monte Carlo, and $P_1$ for an optically thin case with $\tau = 0.1$. The percentage errors in the heat fluxes (compared to Monte Carlo) for the two outer walls are shown in figures 4.27 and 4.28. The results show that the errors in CADOM as well as in the hybrid $S_N - P_N$ are generally quite small, and the largest errors (of about 7% in the outer wall) are confined to the corners. The % errors for the inner walls, in Fig. 4.33 and 4.34 were found to be much lower (of about 2%). It is worth noting that even though 184 million rays were traced, the standard deviation of the Monte Carlo results is about 4%, which renders the errors by the two deterministic methods well within the $\pm 3\sigma$ limit. Similar to the observation made in the 2D geometries, it can be seen that the $P_1$ approximation is inaccurate in the optically thin regime. This is because the $P_1$ approximation does not capture the variation of intensity in the polar and azimuthal directions effectively as it uses only 2 terms in the polynomial expansion of $I$.  

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Figure 4.35: Test Case 3, Heat flux contours on hot outer bottom wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.36: Test Case 3, Heat flux contours on hot outer bottom wall - Monte Carlo and $P_1$ for $\tau_h = 1.0$
Figure 4.37: Test Case 3, Heat flux contours on cold outer back wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.38: Test Case 3, Heat flux contours on cold outer back wall - Monte Carlo and $P_1$ for $\tau_h = 1.0$
Figure 4.39: Test Case 3, Percent errors with Monte Carlo for hot outer bottom wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.40: Test Case 3, Percent errors with Monte Carlo for cold outer back wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$
Figure 4.41: Test Case 3, Heat flux contours on hot inner top wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.42: Test Case 3, Heat flux contours on hot inner top wall - Monte Carlo and $P_1$ for $\tau_h = 1.0$
Figure 4.43: Test Case 3, Heat flux contours on cold inner front wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.44: Test Case 3, Heat flux contours on cold inner front wall - Monte Carlo and $P_1$ for $\tau_h = 1.0$
Figure 4.45: Test Case 3, Percent errors with Monte Carlo for hot inner top wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$

Figure 4.46: Test Case 3, Percent errors with Monte Carlo for cold inner front wall - CADOM and $S_N - P_N$ for $\tau_h = 1.0$
Figure 4.47: Test Case 3, Heat flux contours on hot outer bottom wall - CADOM and $S_N - P_N$ for $\tau_h = 10.0$

Figure 4.48: Test Case 3, Heat flux contours on hot outer bottom wall - Monte Carlo and $P_1$ for $\tau_h = 10.0$
Figure 4.49: Test Case 3, Heat flux contours on cold outer back wall - CADOM and $S_N - P_N$ for $\tau_h = 10.0$

Figure 4.50: Test Case 3, Heat flux contours on cold outer back wall - Monte Carlo and $P_1$ for $\tau_h = 10.0$
Figure 4.51: Test Case 3, Heat flux contours on hot inner top wall - CADOM and $S_N - P_N$ for $\tau_h = 10.0$

Figure 4.52: Test Case 3, Heat flux contours on hot inner top wall - Monte Carlo and $P_1$ for $\tau_h = 10.0$
The figures 4.41, 4.42, 4.43, and 4.44 show the heat flux contours on the outer and inner walls for the case of intermediate optical thickness $\tau_h = 1.0$. From the error plots, it can be inferred that the average error for both CADOM and the hybrid $S_N - P_N$ methods still remain quite small, while the maximum error increases significantly (about 25% for CADOM and 16% for the hybrid $S_N - P_N$ in the outer walls). However, these errors are confined to small regions. The percentage errors observed for the inner walls are still very small with a maximum of around 1%. The standard deviation of the Monte Carlo results in this case was about 7% with considerable statistical noise, making it difficult to compare the accuracy of the CADOM and the $S_N - P_N$ methods. It should be noted that the $P_1$ method still produces unphysical results for the $\tau_h = 1.0$ case.
As the medium becomes optically thicker, the accuracy of the results predicted by $P_1$ approximation improves. This is because the medium becomes more “diffuse” and the use of the $P_1$ approximation is justified. This can be seen from the contour plots in figures 4.47, 4.48, 4.49, and 4.50 for the outer walls. for the optically thick case with $\tau_h = 10.0$. The results obtained with CADOM and the hybrid $S_N - P_N$ compare reasonably well with those from $P_1$. This is along expected lines as the $P_1$ component becomes dominant in optically thick regimes for the hybrid solver. Although Monte Carlo calculations were conducted for the optically thick case, the results were found to be very noisy with standard deviations of about 26%. Therefore, the errors between the Monte Carlo and the other methods are not presented for this case.
Test Case 4

The next test case that was used to test the accuracy of the hybrid $S_N - P_N$ solver was an L-shaped geometry as shown below. The distances shown in Fig. 4.55 are non-dimensionalized with respect to the size of the dimension of the cross-section, and so are all the length dimensions in every figure in this section. The mesh used had 52000 tetrahedral cells.

![L-shaped Geometry Schematic](image1)
![L-shaped Geometry](image2)

(a) L-shaped Geometry Schematic  (b) L-shaped Geometry

Figure 4.55: Test Case 4, L-shaped geometry

The hot walls are kept at $T_h = 1000$ K, the cold walls at 300 K, and the medium temperature is at 300 K. Calculations were performed for both black and reflecting walls with $\epsilon = 0.5$. The heat fluxes and differences in heat fluxes shown in this section are non-dimensionalized with respect to $\sigma(T_h^4 - T_c^4)$. The primary aim of this test case was to test the hybrid solver for cases with both absorption and/or scattering by
the media. Three different conditions with varying scattering albedo were considered and the results are compared with the results from CADOM for different optical thicknesses of the medium, $\tau_h = 0.1, 1.0$ and $10.0$.

- $\omega=0.0$ - Purely Absorbing
- $\omega=0.5$ - Both Absorbing and Scattering
- $\omega=1.0$ - Purely Scattering

![Figure 4.56: Test Case 4, Heat flux contours along back wall of L-shaped geometry, $\omega = 0.0$ for $\tau_h = 1.0$](image)

Three representative heat flux contour plots along the cold top wall and hot back wall are presented here, for a medium with an intermediate optical thickness of $\tau_h = 1.0$. It can be seen from the contour plots that the CADOM and the hybrid
Figure 4.57: Test Case 4, Heat flux contours along top wall of L-shaped geometry, $\omega = 0.0$ for $\tau_h = 1.0$

Figure 4.58: Test Case 4, Heat flux contours along back wall of L-shaped geometry, $\omega = 0.5$ for $\tau_h = 1.0$
Figure 4.59: Test Case 4, Heat flux contours along top wall of L-shaped geometry, \( \omega = 0.5 \) for \( \tau_h = 1.0 \)

Figure 4.60: Test Case 4, Heat flux contours along back wall of L-shaped geometry, \( \omega = 1.0 \) for \( \tau_h = 1.0 \)
Figure 4.61: Test Case 4, Heat flux contours along top wall of L-shaped geometry, $\omega = 1.0$ for $\tau_h = 1.0$

$S_N - P_N$ results match reasonably well for all the scenarios. The maximum percentage difference between the solutions obtained by both these methods for the case with gray walls was found to be 6.1% and 4.3% with reflecting walls for an intermediate optical thickness. A performance study was done for the CADOM and the hybrid $S_N - P_N$ methods, which is discussed in the next section.

Test Case 5

The next test case that was considered was that of the L-shaped geometry used in Test Case 4, with all cold walls and a hot non-homogeneous medium. The walls were at an emissive power of 0.25, while the medium was at unity emissive power. All the walls were assumed to be black. The extinction coefficient was described by
the following relation,

\[
x \leq -y : \beta = \frac{0.9(1.5 + x)(1 - 2|y|)(1 - 2|z|)}{1.5 - y} + 0.1
\]

\[
x < -y : \beta = \frac{0.9(1 - 2|x|)(2.5 - y)(2.5 + x)}{1.5 - y} + 0.1
\]  \hspace{1cm} (4.3)

The comparison of the non-dimensional heat flux [43] along the centerline of the inner front face, as shown in Fig. 4.62 with a scattering albedo of \( \omega = 0.0 \) is shown in Fig. 4.63. The figure shows that the hybrid results do not exactly match with that of the Monte Carlo predictions even though the medium is optically thin. In the previous cases, high accuracy was obtained since the heat flux was dominated by the wall related heat flux due to hot walls. However, in this case, since all the walls are cold, the wall related heat flux is negligible. Hence, the answer is now dominated by the medium related component irrespective of the optical thickness, leading to inaccurate results. Improvement in accuracy can be expected by using a higher order approximation for the solving the medium component, such the \( P_3 \) approximation.
This test case highlights that even though the proposed hybrid method is accurate for most scenarios, there are certain situations in which the basic intensity splitting philosophy becomes redundant, and, consequently, ineffective.

**Test Case 6**

The final test case considered is that of a non-gray emitting-absorbing-scattering medium confined within a three-dimensional L-shaped enclosure. The geometry used in this case, is similar to that used in Test Case 4, with the dimensions of the geometry now being in cm. The rationale behind choosing this test case is to demonstrate
the hybrid solver for a non-gray medium. Also, since non-gray calculations are usually expensive, this particular test case is appropriate for investigating computational efficiency of the proposed hybrid solver especially in comparison to the CADOM. To add further complexity to the problem, the walls were assumed to be reflecting in this case (with gray emissivity, \( \epsilon = 0.5 \)). In the hybrid method, even though directional coupling is absent inside the medium for the wall component of the intensity, the direction equations are still coupled at reflecting boundaries. Thus, a case with reflecting walls represents the worst-case scenario for the hybrid method in terms of computational efficiency. The medium considered in this test case is comprised of 100% Carbon-Dioxide mixed with a background particulate medium. This background medium was considered gray, and its absorption and scattering coefficients were varied to vary the overall optical thickness. The carbon-dioxide, on the other hand, provided the spectral character to the medium. The step-wise gray model that was used to represent the spectrum consisted of three boxes, corresponding to the three primary absorption-emission bands of \( CO_2 \). The width of the boxes (\( \Delta \eta_k \)) and their heights (\( \kappa_k \)) were evaluated at 1700 K from wide-band data following the procedure described by Modest and Sikka [42]. The following values were used for the calculations: \( \kappa_1 = 4.5 \, m^{-1}, \kappa_2 = 90.7 \, m^{-1}, \) and \( \kappa_3 = 17.9 \, m^{-1}, \lambda_1 = 2.7 \, \mu m, \lambda_2 = 4.3 \, \mu m, \) and \( \lambda_3 = 15.0 \, \mu m, \Delta \eta_1 = 445.3 \, cm^{-1}, \Delta \eta_2 = 377.6.3 \, cm^{-1}, \) and \( \Delta \eta_3 = 329.7 \, cm^{-1}. \) The medium was assumed to have a constant temperature of 1700 K. All walls were assumed to be at 1000 K, except the three vertical walls aligned to the Y-Z plane, which were prescribed to be at 2000 K. The background absorption coefficient, \( \kappa_b \), was varied between 1 \( m^{-1} \), and 100 \( m^{-1} \), and the background scattering albedo, \( \omega_{bg} \), was varied between 0 and 1.0. Since the characteristic length scale
in this test case is 1 cm, these values result in the spectral optical thickness varying between 0.2 and 1.1, the most critical range for evaluation of the hybrid method. The computations were performed on an unstructured mesh with 58,000 tetrahedral cells.

Figure 4.64: Test Case 6, Non-dimensional heat flux contours along top wall - CADOM - $\kappa_b = 10$, $\omega_{bg} = 0.5$

Figure 4.65: Test Case 6, Non-dimensional heat flux contours along top wall - hybrid $S_N P_N$ - $\kappa_b = 10$, $\omega_{bg} = 0.5$
Figures 4.64 and 4.65 show the non-dimensional radiative heat flux on the bottom wall (X-Y plane) for $\omega_{bg} = 0.5$ and $\kappa_b = 10 \text{ m}^{-1}$. It is clear from both these figures that the results of the new hybrid method and the standard CADOM are quite similar. Since no Monte Carlo results are available for this test case, it is not possible to assess the accuracy of either method quantitatively. The main purpose of choosing this test case, however, was to study the computational efficiency of the hybrid $S_N - P_N$ method, and these results are discussed next.

4.3 Performance Studies

So far, the accuracy of the hybrid solver has been investigated. The following section presents a comparison of the run times taken by the hybrid $S_N P_N$ solver and CADOM solver for the different test cases.

<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$\tau_h$</th>
<th>CADOM (min)</th>
<th>Hybrid (min)</th>
<th>Improvement Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.1</td>
<td>13.19</td>
<td>4.33</td>
<td>3.04</td>
</tr>
<tr>
<td>0</td>
<td>1.0</td>
<td>12.76</td>
<td>3.89</td>
<td>3.28</td>
</tr>
<tr>
<td>0</td>
<td>10.0</td>
<td>30.82</td>
<td>8.33</td>
<td>3.70</td>
</tr>
<tr>
<td>0.5</td>
<td>0.1</td>
<td>14.68</td>
<td>4.59</td>
<td>3.20</td>
</tr>
<tr>
<td>0.5</td>
<td>1.0</td>
<td>21.53</td>
<td>3.98</td>
<td>5.41</td>
</tr>
<tr>
<td>0.5</td>
<td>10.0</td>
<td>30.81</td>
<td>2.59</td>
<td>11.86</td>
</tr>
<tr>
<td>1.0</td>
<td>0.1</td>
<td>15.04</td>
<td>3.21</td>
<td>4.68</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>31.39</td>
<td>2.84</td>
<td>11.04</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>201.55</td>
<td>2.59</td>
<td>77.53</td>
</tr>
</tbody>
</table>

Table 4.2: Timing studies for Test Case 3 with $\epsilon = 1.0$
All computations were performed on an Intel Core 2 Duo, with 2.3 GHz processor speed and 3.23 GB memory. Quantitative comparison of the difference in computational performance of the CADOM and the hybrid CADOM-$P_1$ methods are provided in this section. The computational times reported are for 10 orders of magnitude decrease in the residuals ($l_2$ norm) of all directional equations and the $P_1$ equation (in the case of the hybrid method).

<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$\tau_h$</th>
<th>CADOM (min)</th>
<th>Hybrid (min)</th>
<th>Max. % Error</th>
<th>Improvement Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.1</td>
<td>40.63</td>
<td>31.40</td>
<td>0.05</td>
<td>1.30</td>
</tr>
<tr>
<td>0</td>
<td>1.0</td>
<td>31.86</td>
<td>24.15</td>
<td>0.09</td>
<td>1.31</td>
</tr>
<tr>
<td>0</td>
<td>10.0</td>
<td>17.44</td>
<td>11.98</td>
<td>0.075</td>
<td>1.46</td>
</tr>
<tr>
<td>0.5</td>
<td>0.1</td>
<td>42.79</td>
<td>31.37</td>
<td>0.901</td>
<td>1.36</td>
</tr>
<tr>
<td>0.5</td>
<td>1.0</td>
<td>41.86</td>
<td>24.15</td>
<td>1.7</td>
<td>1.73</td>
</tr>
<tr>
<td>0.5</td>
<td>10.0</td>
<td>34.22</td>
<td>12.07</td>
<td>0.59</td>
<td>2.83</td>
</tr>
<tr>
<td>1.0</td>
<td>0.1</td>
<td>42.74</td>
<td>31.56</td>
<td>1.81</td>
<td>1.35</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>53.82</td>
<td>24.15</td>
<td>4.31</td>
<td>2.23</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>139.10</td>
<td>12.01</td>
<td>3.81</td>
<td><strong>11.58</strong></td>
</tr>
</tbody>
</table>

Table 4.3: Timing studies for Test Case 4 with $\epsilon = 0.5$

<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$\tau_h$</th>
<th>CADOM (min)</th>
<th>Hybrid (min)</th>
<th>Max. % Error</th>
<th>Improvement Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.1</td>
<td>11.45</td>
<td>8.30</td>
<td>0.036</td>
<td>1.38</td>
</tr>
<tr>
<td>0</td>
<td>1.0</td>
<td>11.27</td>
<td>7.93</td>
<td>0.482</td>
<td>1.42</td>
</tr>
<tr>
<td>0</td>
<td>10.0</td>
<td>10.21</td>
<td>6.76</td>
<td>0.09</td>
<td>1.51</td>
</tr>
<tr>
<td>0.5</td>
<td>0.1</td>
<td>12.08</td>
<td>8.47</td>
<td>1.71</td>
<td>1.43</td>
</tr>
<tr>
<td>0.5</td>
<td>1.0</td>
<td>15.18</td>
<td>7.91</td>
<td>0.99</td>
<td>1.92</td>
</tr>
<tr>
<td>0.5</td>
<td>10.0</td>
<td>25.93</td>
<td>6.72</td>
<td>1.52</td>
<td>3.86</td>
</tr>
<tr>
<td>1.0</td>
<td>0.1</td>
<td>12.40</td>
<td>8.41</td>
<td>0.48</td>
<td>1.47</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>19.16</td>
<td>7.96</td>
<td>2.09</td>
<td>2.41</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>69.44</td>
<td>6.71</td>
<td>6.13</td>
<td><strong>10.40</strong></td>
</tr>
</tbody>
</table>

Table 4.4: Timing studies for Test Case 4 with $\epsilon = 1.0$
\[
\begin{array}{|c|c|c|c|c|}
\hline
\omega_{bg} & k_b & \text{CADOM (min)} & \text{Hybrid (min)} & \text{Improvement Factor} \\
\hline
0 & 1.0 & 137.62 & 109.81 & 1.25 \\
0 & 10.0 & 127.83 & 100.24 & 1.28 \\
0 & 100.0 & 87.04 & 67.04 & 1.30 \\
0.5 & 1.0 & 164.93 & 111.49 & 1.48 \\
0.5 & 10.0 & 162.98 & 100.88 & 1.62 \\
0.5 & 100.0 & 153.76 & 67.27 & 2.29 \\
1.0 & 1.0 & 208.82 & 111.06 & 1.90 \\
1.0 & 10.0 & 218.62 & 101.49 & 2.15 \\
1.0 & 100.0 & 341.08 & 67.67 & 5.04 \\
\hline
\end{array}
\]

Table 4.5: Timing studies for Test Case 6 with \( \epsilon = 0.5 \)

\[
\begin{array}{|c|c|c|c|c|}
\hline
\omega_{bg} & k_b & \text{CADOM (min)} & \text{Hybrid (min)} & \text{Improvement Factor} \\
\hline
0 & 1.0 & 35.49 & 26.36 & 1.35 \\
0 & 10.0 & 34.85 & 25.82 & 1.36 \\
0 & 100.0 & 31.47 & 21.95 & 1.43 \\
0.5 & 1.0 & 69.72 & 26.80 & 2.60 \\
0.5 & 10.0 & 80.82 & 25.88 & 3.12 \\
0.5 & 100.0 & 100.21 & 21.99 & 4.56 \\
1.0 & 1.0 & 120.84 & 27.14 & 4.45 \\
1.0 & 10.0 & 142.14 & 26.24 & 5.42 \\
1.0 & 100.0 & 354.07 & 22.55 & 15.70 \\
\hline
\end{array}
\]

Table 4.6: Timing studies for Test Case 6 with \( \epsilon = 1.0 \)

The above tabulated results clearly show that the proposed new hybrid method is superior to the standard CADOM in terms of computational efficiency for all cases. The minimum improvement factor is 1.3, which is found to be manifested in the case when the medium is non-scattering and the walls are reflecting. This is because, in this case, the directional equations in standard CADOM become decoupled, and its performance is closer to that of the hybrid method. On the other hand, for strongly
scattering medium with black walls, the computational gains provided by the hybrid method over standard CADOM are found to be more than an order of magnitude. The hybrid method manifested gains of close to a factor of 100 for scattering dominant gray cases with large optical thickness (Table 4.2). It is observed that for the cases with reflecting walls, the improvement factor is lower because of the coupling of the intensity equations at the boundaries for the hybrid solver. Based on these results, it is fair to contend that the hybrid method is favorable over standard CADOM as a general-purpose RTE solver since it provides similar accuracy at a much lower computational cost.
The challenges involved in the accurate numerical solution of the radiative transfer equation (RTE) were briefly discussed in Chapter 1. The two most popular methods that are currently in use for the numerical solution of the RTE are the method of spherical harmonics ($P_N$ Approximation) and the discrete ordinates method ($S_N$ Approximation). However, both these methods have their own shortcomings and there is still the lack of a general-purpose, efficient solution method that yields accurate results for all optical thickness. The main objective of this thesis was to formulate a new, robust, computationally efficient hybrid method that addresses this long-standing need.

In the proposed hybrid method, the philosophy of splitting of radiant intensity into a “wall” component and a “medium” component, as in the Modified Differential Approximation (MDA), was employed. The wall-emitted component accounts for ballistic transport, i.e., wall-to-wall radiation transport, while the “medium” component accounts for the diffusive medium-wall interaction. In earlier attempts to solve the RTE using the MDA approximation, the wall-emitted component was computed
using a view-factor based surface to surface exchange formulation, and the “medium” component was solved using the $P_1$ approximation. Though this approach yielded good accuracy over a large range of optical thickness, the computation of the view-factors, and, subsequently, storing them for complex 3D geometries, proved to be a major bottleneck both from a computational efficiency and memory standpoint. This led to the pursuit of the hybrid $S_N - P_N$ scheme that was developed in this work.

In the hybrid $S_N - P_N$ scheme, the ballistic component is determined using the Discrete Ordinates Method. The main advantage of this method is that the directional equations for the wall component of intensity, unlike those for the total intensity in the discrete ordinates method, are no longer coupled. This resulted in huge gains in computational efficiency since no iterations are necessary because of the absence of directional coupling. However, the standard discrete ordinates method suffered from “ray effects” and “false scattering”, and hence, a variant of this method, namely, the Control Angle Discrete Ordinates Method (CADOM), was also developed and implemented for determining the wall component. The “medium” component was solved using the $P_1$ approximation. A finite-volume procedure was used to discretize the governing equations. The resulting set of linear algebraic equations were solved on an unstructured mesh using the ILU-preconditioned GMRES solver.

The accuracy of this hybrid method was evaluated by comparing the results with those obtained using CADOM, $P_1$ approximation, and Monte Carlo method, all of which were developed as part of this thesis. The medium thickness was varied by three orders of magnitude.
It was found that for optically thick cases, all the methods gave accurate results when compared to the “exact” Monte Carlo solutions. For optically thin situations, the $P_1$ method showed poor accuracy predicting unphysical results in some regions, while the results from CADOM and the hybrid $S_N - P_N$ method matched exactly with the Monte Carlo results. Least accuracy was obtained for the intermediate optical regime, wherein, the final solution was affected by both the components, but was still considerably better than $P_1$. The errors in this scenario were comparable to those obtained with CADOM, which, incidentally, was the most accurate among several other existing methods that were explored.

The main noteworthy advantage of the proposed hybrid $S_N - P_N$ method is the computational gains realized. To assess the efficiency of this method, the hybrid solver was explored for a three-dimensional enclosure containing a non-gray absorbing-emitting-scattering gas-particulate mixture and having reflecting walls. For all parametric variations considered, the hybrid method was found to be at least 30% more efficient than the standard control angle discrete ordinates method, and up to 15 times computationally more efficient than the control angle discrete ordinates method for cases that have large optical thickness and/or strong scattering. In the same geometry with a gray medium, the hybrid method was found to be as much as 100 times more efficient than the CADOM. Based on these comprehensive studies, it is believed that the proposed hybrid $S_N - P_N$ solver holds strong potential as an RTE solver since it is able to produce accurate results over a wide range of optical thickness at a computational cost much smaller than the most popular RTE solvers currently in use.
It should be noted that the hybrid $S_N - P_N$ method developed in this work, although found to be accurate for the vast majority of problems tested, has its own shortcomings. In a scenario dominated by medium emission, with negligible contribution from wall-to-wall transport (as in the case of cold walls enclosing a hot optically thin medium), this method shows poor accuracy. In this case, the “medium” component of the solver is the only component that affects the solution, and since the 1st order $P_1$ approximation is used to solve for the medium component, the results exhibit poor accuracy. In order to improve the accuracy of this method in such scenarios, one avenue to pursue would be to apply the $S_N - P_N$ approximation to a higher order $P_N$ approximation, such as the $P_3$ approximation, for obtaining a more accurate solution to the “medium” component.

In order to conclusively demonstrate the efficacy of the hybrid method, it needs to be tested for real-life problems with real non-gray properties. This implies integration with state-of-the-art spectral models such as the Full-Spectrum Correlated k-Distribution (FSCK) model [44] and the Spectral Line-Weighted (SLW) model [45, 46]. This is one direction for future work.

In order to further improve the computational efficiency of the hybrid RTE method, one might look at parallelizing the existing non-gray solver. This can be done with relative ease as the directional intensity equations for the wall - emitted component are now decoupled. Finally, the RTE solver needs to be coupled with the overall energy equation (CFD solver) to assess its performance.


