

Monte Carlo Radiative Transfer Approach to determine BRDF for airless planetary surfaces

SUMMER PROJECT REPORT

May 24' - July 24'

Submitted by

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Integrated M.Sc. 2020-2025

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July 15th, 2024



ACKNOWLEDGEMENT

I would like to express my special sense of gratitude to my supervisor, **Dr. Megha Bhatt** (PSDN-PRL) for her invaluable guidance towards the project. Without her involvement and persistent support, this project would not have been possible. I am extremely grateful to **Dr. Mauro Ciarniello** (IAPS-INAF, Italy) for providing his invaluable feedback on reaching out to him when required. I would also like to thank **Ms. Sachana A S** (PhD Scholar, PSDN-PRL) and **Mr. Dibyendu Misra** (PhD Scholar, PSDN-PRL), for their constant help, support and beneficial advice that guided me throughout and helped me at times of doubts. I am also thankful to **Mr. Prajul Adhikari** (MSc, NIT Silchar) for helping me with his experience whenever I needed.

I would extend my appreciation to the Chairperson, UGC of SPS, NISER and Academics Head, PRL for providing me an opportunity to undertake this project. I am grateful to the staff and faculty at **PRL, Ahmedabad**, who managed this summer programme successfully and helped me throughout. I would also like to thank my parents, sisters and friends whose encouragement made the biggest difference.

This project gave me a great learning experience with simulations and I developed many personal qualities throughout like responsibility, punctuality, confidence, perseverance and dedication. I thank all the individuals and institutions mentioned above, as well as to anyone else who has directly or indirectly contributed to this project. Their contributions have played a significant role in the successful completion of this research, and I am truly grateful for their support.

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ABSTRACT

This report presents a comprehensive study on the application of MCRT methods to derive physical properties from reflectance spectra of airless planetary bodies. Reflectance spectroscopy is a crucial tool in planetary science for understanding surface compositions and physical characteristics. While traditional models like Hapke's provide significant insights, they have limitations such as assumptions and inability to accurately account for complex scattering behaviors in heterogeneous or anisotropic media that can be addressed by more appropriate models. The primary objective of this project is to compare direct and indirect MCRT approaches and evaluate their potential for deriving physical properties from reflectance spectra obtained through remote sensing, particularly for data from the Chandrayaan mission.

The methodology involves simulating the interaction of light with particulate surfaces and comparing the outcomes of both MCRT approaches i.e. Direct and Indirect. Results were expected to indicate that MCRT methods offer improved accuracy and efficiency over conventional techniques, providing a robust tool for analyzing remote sensing data. This report details the theoretical background, model development and simulation setup, highlighting the potential applications of the MCRT model in planetary science and remote sensing.

Initially, the project reproduces reference study results, focusing on the influence of the filling factor (ϕ) on a simulated particulate medium's reflectance. The effects of ϕ and single scattering albedo (SSA) on the reflectance curve were successfully obtained, supporting the MCRT method's capability to model these parameters accurately. Both direct and indirect MCRT methods were developed and implemented, revealing distinct differences in reflectance values that underscore the importance of proper normalization.

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Chapter 1

Introduction

1.1 Overview

Reflectance spectroscopy is a pivotal analytical technique in planetary science, enabling the determination of the composition and physical properties of planetary surfaces. By analyzing the light reflected from these surfaces, scientists can infer a wealth of information about the mineralogical makeup, texture, and other essential characteristics. This method is particularly vital for studying airless planetary bodies such as the Moon, asteroids, and Mercury. These celestial objects lack an atmosphere, allowing for a clearer and more direct interpretation of the spectral data without the complicating effects of atmospheric interference.

Traditionally, models such as the Hapke model [Hapke, 2012] have been widely used to interpret reflectance spectra. Hapke's model offers a comprehensive framework for understanding the scattering of light in particulate surfaces and has been instrumental in numerous planetary studies [Shepard and Helfenstein, 2011, Stankevich and Shkuratov, 2004, Ciarniello et al., 2011]. However, it relies on several simplifying assumptions and approximations, which can limit its accuracy under certain conditions [Shepard and Helfenstein, 2007]. To overcome these limitations and achieve a more precise understanding of reflectance spectra, advanced computational approaches like the Monte Carlo Radiative Transfer (MCRT) method are increasingly being explored. [Stankevich and Shkuratov, 2004, Ciarniello et al., 2019]

The MCRT method stands out for its ability to simulate the complex interactions of photons with particulate media in a statistically rigorous manner. By tracing the paths of a large number of photons as they scatter and absorb within the medium, MCRT can provide highly accurate predictions of reflectance spectra. This method is particularly effective in handling the complexities of multiple scattering events, which are often challenging to model accurately with analytical methods like the Hapke model.

In the following sections, we will delve into the theoretical foundations of the MCRT method, describing the underlying physics and mathematical formulations. We will then outline the development and implementation of both direct and indirect MCRT models, including details on the algorithms based on the routine given in Ciarniello et al., 2014, computational techniques, and validation

processes used. This will be followed by a presentation of the simulation results, where we will compare the performance and accuracy of the direct and indirect MCRT methods. Finally, we will discuss the potential applications of the developed MCRT tool in planetary science, highlighting its advantages, limitations, and areas for future improvement.

Ultimately, this work aims to enhance the accuracy and utility of reflectance spectroscopy in studying planetary surfaces. By providing a robust and efficient tool for generating reflectance spectra, we hope to contribute to the broader field of planetary science, facilitating more accurate interpretations of remote sensing data and advancing our understanding of the composition and physical properties of planetary bodies.

1.2 Objective

This report focuses on the development of the MCRT method in order to derive physical properties from reflectance spectra using this model. Due to time constraints, the project has been limited to exploring the MCRT approach, without making direct comparisons to the Hapke model. The primary objective of this work is to develop and validate both direct and indirect MCRT methods. These methods aim to create a tool that can efficiently and accurately generate reflectance spectra, which can then be applied in various planetary science contexts.

The direct MCRT method involves simulating the precise paths of individual photons as they interact with the medium, tracking each scattering and absorption event. This approach, while highly accurate, can be computationally intensive due to the need to simulate a large number of photon interactions to achieve statistically significant results. The indirect MCRT method, on the other hand, introduces efficiencies by using probabilistic models to estimate the overall distribution of photon interactions within the medium, reducing the computational burden while still maintaining a high level of accuracy.

Chapter 2

Theoretical Background

2.1 Radiative Transfer

Radiative transfer theory forms the foundation of understanding how light interacts with materials, which is essential for interpreting reflectance spectra in planetary science. The basic principles of radiative transfer involve the propagation of electromagnetic radiation through a medium, considering absorption, scattering, and emission processes. These interactions determine the intensity and spectral distribution of the light that ultimately reaches an observer.

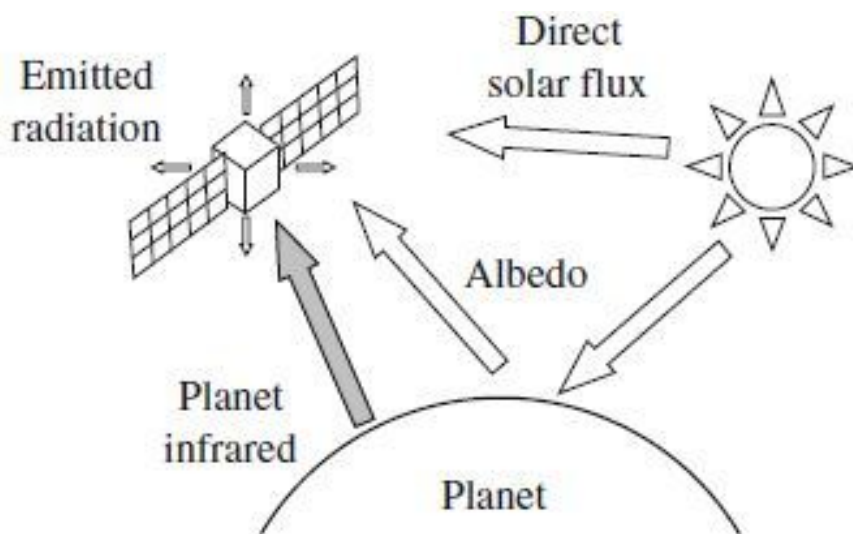


Figure 2.1: Radiation transfer for a remote sensing satellite in space environment [Nogueira, 2017]

In planetary science and remote sensing, radiative transfer theory is crucial for decoding the information contained in reflected light from planetary surfaces. By analyzing how light is absorbed and scattered by surface materials, we can infer the composition, texture, and other physical properties of these surfaces. This theoretical framework allows for the development of models that can predict how light will behave when it interacts with various materials, providing a basis for interpreting remote sensing data from planetary bodies. [Kato and Fukue, 2020]

In the context of this paper, radiative transfer is essential for understanding and modeling the reflectance spectra of planetary surfaces. Hapke's model is a widely used analytical approach to solving the radiative transfer equation for particulate surfaces, particularly in planetary science. MCRT uses statistical sampling to simulate the paths of photons through a medium, allowing for the modeling of complex interactions, including anisotropic scattering and heterogeneous media. By tracking individual photons and their interactions with particles, MCRT can account for detailed geometric and physical properties of the medium, providing a more accurate approximation of the reflectance spectra. In particular, it is employed to simulate these interactions in a statistically rigorous manner since it uses statistical sampling to solve the Radiative Transfer Equation (RTE) by simulating the paths of many photons as they interact with the medium.

2.2 Hapke Model

The Hapke model is a most widely used analytical approach for modeling the reflectance of particulate surfaces, particularly those found on airless planetary bodies. Developed by Bruce Hapke, this model accounts for several key factors that influence reflectance, including single scattering albedo, phase function, surface roughness, and porosity of the material.

Key equations in the Hapke model include those describing the bidirectional reflectance function (BRDF), which defines how light is reflected at different angles, and the opposition effect like Shadow Hiding Opposition effect (SHOE) and Coherent Backscattering Opposition Effect (CBOE), which explains the increase in brightness observed when the phase angle approaches zero. The model also incorporates the effects of multiple scattering, where photons are scattered more than once before exiting the surface. [Shepard and Helfenstein, 2011]

The Hapke model [Hapke, 2012] describes the bidirectional reflectance function (BDRF) depending on the incident and emitted light directions. The reflectance function is given by:

$$r(i, e, g) = K \frac{w}{4\pi} \frac{\mu_0 e}{\mu_0 e + \mu_e} \left[(1 + B_{SH}(g))p(g) + M\left(\frac{\mu_0 e}{K}, \frac{\mu_e}{K}, g\right) \right] (1 + B_{CB}(g))S(\mu_0 e, \mu_e, \psi) \quad (2.1)$$

The key variables in these models include w , the single scattering albedo, K , the porosity correction factor, g , the phase angle, $\mu_0 e$, the effective cosine of the incidence angle, μ_e , the effective cosine of the emission angle, B_{SH} representing the shadow hiding opposition effect, B_{CB} representing the coherent backscatter opposition effect, $S(\mu_0 e, \mu_e, \psi)$ which accounts for shadowing on rough surfaces depending on the azimuth angle ψ , $M(\mu_0 e/K, \mu_e/K, g)$ which models multiple scattering, ϕ which is the filling factor representing the fraction of the volume occupied by particles, and b and c which are empirical parameters determining the shape and strength of scattering lobes. [Refer to 4.2 for terms and abbreviations]

Porosity affects light scattering, with denser materials behaving differently from porous ones. K is calculated as:

$$K = -\frac{\ln\left(1 - 1.209\phi^{\frac{2}{3}}\right)}{1.209\phi^{\frac{2}{3}}} \quad (2.2)$$

The phase function $p(g)$ describes light scattering by individual particles and is given by the double-lobed Henyey-Greenstein function:

$$p(g) = \frac{1+c}{2} \left(\frac{1-b^2}{(1-2b\cos g + b^2)^{\frac{3}{2}}} \right) + \frac{1-c}{2} \left(\frac{1-b^2}{(1+2b\cos g + b^2)^{\frac{3}{2}}} \right) \quad (2.3)$$

Brightness increases as the phase angle g approaches zero due to the opposition effects:

- SHOE - Shadows are cast by particles blocking the light source. It is quantified by:

$$B_{SH}(g) = \frac{B_0}{1 + \frac{1}{h} \tan\left(\frac{g}{2}\right)} \quad (2.4)$$

where B_0 is the SHOE amplitude and h is related to the filling factor ϕ by:

$$h = -\frac{3}{8} \ln(1 - \phi)$$

- CBOE - Constructive interference of scattered wave fronts enhances brightness at small phase angles. It is generally not taken into account as it only occurs at very small angles.

Multiple scattering is modeled by $M(\mu_0 e/K, \mu_e/K, g)$, while $S(\mu_0 e, \mu_e, \psi)$ accounts for shadowing on rough surfaces. The Chandrasekhar function approximates multiple scattering:

$$H(x, w) = \frac{1 + 2x}{1 + 2\gamma x} \quad (2.5)$$

Now under the assumption of isotropic scattering-

$$\gamma = \sqrt{1 - w}$$

The equation 2.6 is derived from equation 2.1 by simplifying several factors and functions. The constant K and the Chandrasekhar function $B_{CB}(g)$ are normalized out, simplifying the remaining terms. The M function, which accounts for multiple scattering, is approximated by $H(\mu, w)H(\mu_0, w) - 1$, where H represents the Chandrasekhar H-function. The $S(\mu_0 e, \mu_e, \psi)$ term, which accounts for surface roughness and shadowing effects, is similarly absorbed into the H-function approximation. This transformation results in a more streamlined expression for reflectance that emphasizes the core components of single scattering albedo w , phase function $p(g)$, and the angles of incidence and emission.

The Hapke model describes the bidirectional reflectance distribution function (BDRF) based on incident and emitted light directions. The reflectance $r(i, e, g)$ is expressed as:

$$r(i, e, g) = \frac{w}{4\pi \mu_0 e + \mu_e} [(1 + B_{SH}(g))p(g) + H(\mu, w)H(\mu_0, w) - 1] \quad (2.6)$$

where w is the single scattering albedo, μ_0 is the cosine of the incidence angle, μ is the cosine of the emission angle, g is the phase angle, $B_{SH}(g)$ represents the shadow hiding opposition effect

and $p(g)$ is the particle phase function $H(x, w)$ is the Chandrasekhar function given by equation 2.5 is approximated in isotropic medium as:

$$H(x, w) = \frac{1 + 2x}{1 + 2x\sqrt{1 - w}}$$

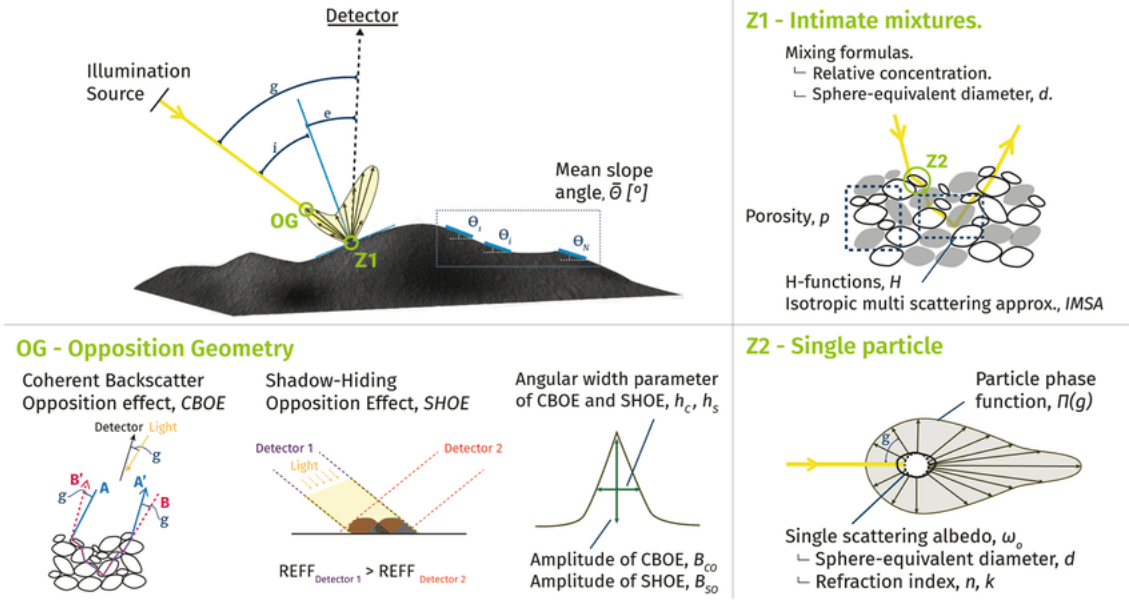


Figure 2.2: Illustration of the Hapke model with the key parameters [Pommerol et al., 2019]

Assumptions in the Hapke model, such as the independence of scattering events and the isotropy of the scattering medium, make it computationally efficient but can limit its accuracy in certain situations. Despite these limitations, the Hapke model remains a cornerstone in planetary reflectance studies due to its comprehensive treatment of various scattering phenomena and its relative simplicity. The three major formulation of the Hapke theory has been often used as references: The Isotropic Multiple Scattering (IMSA) model, the Anisotropic Multiple Scattering (AMSA) Model and Hapke, 2008[H2008] Model.

2.2.1 IMSA Model

The Improved Multiple Scattering Approximation (IMSA) model refines the Hapke model by providing a more accurate description of multiple scattering. The reflectance $r_{IMSA}(i, e, g)$ is given by:

$$r_{IMSA}(i, e, g) = \frac{w\mu_0}{4\pi(\mu_0 + \mu)} [1 + B_{SH}(g)] p(g) + \frac{H(\mu, w)H(\mu_0, w) - 1}{\mu + \mu_0} \quad (2.7)$$

$p(g)$ is defined by equation 2.3

2.2.2 AMSA Model

The Anisotropic Multiple Scattering Approximation (AMSA) model improves upon the IMSA by abandoning the assumption of isotropic scattering, giving a more precise description of the multiple scattering process. The BDRF $r_{AMSA}(i, e, g)$ is:

$$r_{AMSA}(i, e, g) = \frac{w\mu_0}{4\pi(\mu_0 + \mu)} [1 + B_{SH}(g)] p(g) + M(w, \mu_0, \mu) \quad (2.8)$$

where the multiple scattering term $M(w, \mu_0, \mu)$ is given by:

$$M(\mu_0, \mu) = P(\mu_0)[H(\mu) - 1] + P(\mu)[H(\mu_0) - 1] + P[H(\mu) - 1][H(\mu_0) - 1] \quad (2.9)$$

$P(x)$ and P are particular averages of $p(g)$.

2.2.3 Hapke (2008) Model

The 2008 version of the Hapke model incorporates porosity effects. The reflectance $r(i, e, g)$ is given by:

$$r(i, e, g) = \frac{w}{4\pi} \frac{\mu_0 e}{\mu_0 e + \mu_e} [(1 + B_{SH}(g))p(g) + M(w, \mu_0, \mu)] \quad (2.10)$$

where the porosity correction factor K is:

$$K = \frac{-\ln\left(1 - 1.209\phi^{\frac{2}{3}}\right)}{1.209\phi^{\frac{2}{3}}} \quad (2.11)$$

and the multiple scattering term $M(w, \mu_0, \mu)$ is:

$$M(\mu_0, \mu) = P(\mu_0)[H(\mu) - 1] + P(\mu)[H(\mu_0) - 1] + P[H(\mu) - 1][H(\mu_0) - 1] \quad (2.12)$$

In the 2008 model, the effect of opposition is not explicitly included, but it was later introduced in Hapke (2012) with the parameter h for the SHOE being:

$$h = \frac{3K\phi}{8}$$

When the opposition effect is included, the final BDRF expression becomes:

$$r(i, e, g) = \frac{w}{4\pi} \frac{\mu_0 e}{\mu_0 e + \mu_e} [(1 + B_{SH}(g))p(g) + H(\mu_0, w)H(\mu, w) - 1] \quad (2.13)$$

These models collectively provide a framework for understanding the bidirectional reflectance properties of particulate surfaces, accounting for single scattering, multiple scattering, shadowing effects, and porosity. The Hapke model integrates these effects to comprehensively describe light reflectance from particulate surfaces.

This report very briefly deals with the Hapke Model due to time constraints but the purpose of comparing it with the MCRT technique would result in validating the MCRT model as a successful alternate tool for studying other airless planetary surfaces like Moon and Mercury.

2.3 Monte Carlo Radiative Transfer (MCRT) Model

Monte Carlo radiative transfer (MCRT) is a sophisticated numerical technique used to model the propagation of radiation through a medium. This method is particularly valuable in scenarios where the medium is complex, such as in astrophysics, atmospheric science, and medical physics. The fundamental principle of MCRT is the statistical simulation of photon paths, treating radiation as a collection of discrete particles or rays [Noebauer and Sim, 2019]. Each photon or ray is followed as it interacts with the medium through processes such as scattering, absorption, and emission.

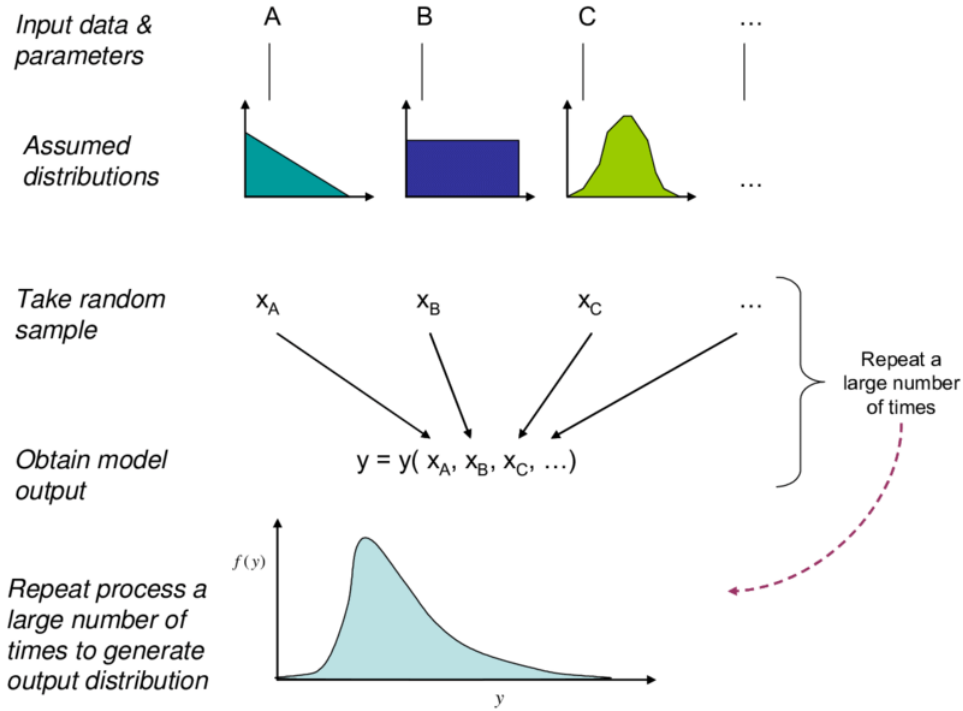


Figure 2.3: Graphical depiction of monte carlo simulation procedure [Henderson and Bui, 2005]

In an MCRT simulation, photons are generated and traced through the medium, with their paths determined by probabilistic rules that reflect the physical properties of the material. The probability of a photon being scattered or absorbed is based on the medium's optical properties, such as its opacity and scattering coefficient. The direction of scattering and the distance a photon travels before an interaction are typically determined using random sampling techniques. This stochastic approach allows for the simulation of complex interactions and the accurate modeling of radiation fields in heterogeneous and anisotropic media.

The MCRT method can accommodate various boundary conditions, such as reflective surfaces or periodic boundaries, and can incorporate detailed models of the medium's optical properties. This makes MCRT particularly useful for applications where exact solutions are difficult or impossible to obtain analytically. Moreover, advances in computational power and algorithm efficiency have made MCRT a practical tool for high-resolution simulations, providing insights into the behavior of radiation in systems with intricate geometries and varying material properties.

The accuracy of the results depends on the number of photons simulated; thus, achieving a balance between computational cost and accuracy is a critical aspect of using this method effectively. Additionally, implementing MCRT requires careful consideration of numerical issues such as variance reduction techniques, which are essential for minimizing statistical noise in the simulation results.

2.3.1 Direct Monte Carlo Radiative Transfer

Direct Monte Carlo radiative transfer (Direct MCRT) focuses on the explicit simulation of photon transport from a radiation source through a medium to a detector. In Direct MCRT, photons are emitted from a defined source and their trajectories are traced as they travel through the medium, undergoing interactions such as scattering and absorption. This method is particularly effective in scenarios where the direct paths of photons and their primary interactions are of interest, such as in imaging or in the study of radiation beams. [Noebauer and Sim, 2019]

Direct MCRT is often employed in applications requiring detailed spatial and angular resolution of the radiation field. In astrophysics, it helps in understanding the direct illumination and shadowing effects in interstellar environments. The primary challenge in Direct MCRT lies in ensuring sufficient photon sampling to achieve accurate results, which can be computationally demanding.

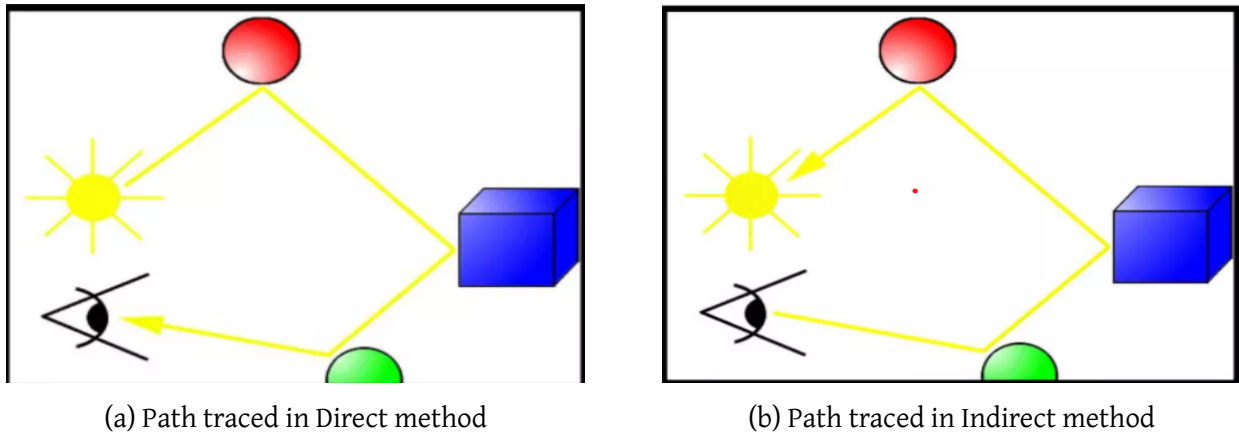


Figure 2.4: Path traced by photons in MCRT [Noebauer and Sim, 2019]

2.3.2 Indirect Monte Carlo Radiative Transfer

Indirect Monte Carlo radiative transfer (Indirect MCRT) emphasizes the treatment of scattered radiation and diffuse light transport within the medium. Instead of focusing solely on the direct paths of photons from the source, Indirect MCRT accounts for the multiple scattering events that photons undergo, which significantly contribute to the overall radiation field. This approach is crucial in environments where scattering dominates, such as in planetary atmospheres or within dense interstellar clouds.

In this method, capturing the complex interplay of multiple scattering events that redistribute the radiation throughout the medium [Noebauer and Sim, 2019]. This technique is vital for accurate simulations of diffuse lighting conditions, where photons may undergo numerous interactions before reaching a detector. When compared to traditional methods like the Hapke model, it does not rely on simplifying assumptions about the independence of scattering events or isotropy, allowing for more accurate modeling of complex surfaces. However, the computational intensity of MCRT can be a drawback, especially for large-scale simulations.

Chapter 3

Methodology

In the MCRT routines, photons or packets of photons are propagated to the medium where they can be absorbed or scattered and the path is traced. By propagating a large number of photon packets, the photometric output of the medium can be reconstructed, described in terms of reflectance $r(i, e, g)$, where i and e are the incidence and emission angles, and g is the phase angle.

3.1 Modelling

The preliminary model of the MCRT Simulation has been reproduced according to the description given in Ciarniello et al., 2014, Ciarniello et al., 2019 Salo and Karjalainen, 2003 and Stankevich and Shkuratov, 2004.

3.1.1 Direct MCRT Method

The Direct MCRT method involves simulating the paths of photon packets as they travel from the light source, through the medium, and towards the detector in the following process:

- **Initialization:** Define the optical properties of the medium, including particle characteristics such as radius, single scattering albedo (SSA), and the single scattering phase function.
- Set up the original positions of the light source.
- **Interaction Probability:** Determine whether the photon is absorbed or scattered based on the SSA. If absorbed, the photon packet is removed from the simulation count. If scattered, the photon's direction is updated using the single scattering phase function $p(g)$.
- Determine the probability of absorption during each interaction. The probability of absorption is $1 - w$, where w is the SSA.
- Compare w to a random variable v_1 uniformly distributed in the range $[0, 1]$. If $v_1 > w$, then absorption occurs, and the photon's journey ends. Otherwise, the photon is scattered.
- If the photon is not absorbed, it is scattered to a new direction determined by a phase angle g . Calculate the probability as $dP(g) = p(g)dX = p(g)2\pi \sin(g)dg$, where $p(g)$ is the single scattering phase function.

- Generate a guess for g and compute $dP(g)/dg = p(g)2\pi \sin(g)$. Compare this value to a random variable v_2 uniformly distributed in the range $[0, \text{MAX}(dP(g)/dg)]$. If $dP(g)/dg > v_2$, then the guessed g is accepted; otherwise, generate a new guess until the condition is satisfied.
- The direction of the scattered photon is fully determined by both the phase angle g and the azimuthal angle ϕ . For spherical particles, scattering does not depend on the azimuth, so $\phi = 2\pi v_3$, where v_3 is a random variable uniformly distributed in the range $[0, 1]$.
- If the photon 'z' position exceeds the slab depth, it is considered to have escaped.
- **Photon Tracking:** Track the photons that escape from the medium and register their directions. Store the properties of the escaped photons.
- Repeat the process for a large number of photon packets (10^7 photons) to ensure statistical accuracy.
- Compute the reflectance scattered in each direction. This is proportional to the ratio between the number of stored scattered photons in that direction and the total number of photons propagated.

3.1.2 Indirect MCRT Method

The Indirect MCRT method, also known as backward ray-tracing, focuses on tracing photon paths from the observer or detector backward through the medium towards the light source. This method is efficient for capturing multiple scattering events and diffuse lighting conditions.

- **Initialization:** Define the optical properties of the medium and the characteristics of the particles.
- **Photon Packet Generation:** Generate photon packets from the observer's direction toward the medium. These packets have initial properties such as energy, direction, and position based on the observer's viewpoint.
- **Photon Propagation:** Propagate the photon packet through the medium, reducing its energy by a factor w (SSA) after each scattering event.
- **Visibility Check:** Check if the photon packet can be traced back to the light source without obstruction. If visible, the photon packet contributes to the total energy reaching the observer.
- **Energy Accounting:** Use the phase angle g_i to compute the energy weight of the photon packet after each scattering event. Accumulate the energy contributions based on the single scattering phase function $p(g_i)$.
- **Multiple Scattering Handling:** Continue propagating the photon packet through multiple scattering events according to the interaction probability similar to the Direct MCRT method until it is either absorbed or leaves the medium. This process ensures that all significant scattering paths are considered.

- Repeat the process for a large number of photon packets (2×10^4 photons) to achieve statistical accuracy.
- Compute the reflectance by averaging the energy of the photon packets reaching the observer. This involves analyzing the cumulative energy and angular distribution of the detected photons.

After n scatterings, the total energy E_m of the m -th photon packet in a given direction is given by:

$$E_m = \sum_{i=1}^n E_0 w^i \frac{P(g_i)}{4\pi} h_i \quad (3.1)$$

where h_i is 0 or 1, indicating whether the photon packet is visible from the source (1 if visible, 0 if not).

The total energy for N photon packets is:

$$E = \sum_{m=1}^N E_m \quad (3.2)$$

This approach ensures accurate calculation of reflectance and photometric properties of the medium.

3.2 Simulation Setup

The medium in this simulation in which scattering takes place has been described as a semi-infinite medium and we approximate it to a slab (box) of spherical-shaped particles. This medium is characterized by several key properties. The depth of the slab is chosen to ensure that light transmission through the medium is sufficiently low, typically less than 1%. This condition ensures that the medium effectively absorbs and scatters most of the incoming light, mimicking the behavior of a semi-infinite medium. Additionally, the medium is defined by a filling factor, which represents the volume fraction of the slab occupied by particles. This factor is crucial in determining the optical density and interaction properties of the medium.

The particles within the medium are assumed to be of uniform size and spherical in shape. This uniformity simplifies the calculations and allows for the use of well-established scattering theories to describe the interaction of light with the particles. The single scattering albedo (SSA) represents the probability that a photon will be scattered rather than absorbed during an interaction. A high SSA indicates that scattering is the dominant interaction process, while a low SSA suggests significant absorption. Furthermore, the single scattering phase function, typically derived from the Henyey-Greenstein Function [Henyey and Greenstein, 1941] for spherical particles, describes the angular distribution of scattered light.

In the MCRT simulations, periodic boundary conditions are applied to approximate a semi-infinite medium with finite horizontal extension. These conditions ensure that the simulation accurately represents the behavior of photons in an unbounded medium. Periodic boundary conditions help

maintain the statistical consistency of photon interactions by avoiding the artificial loss of photons at the domain edges. This approach ensures that all photons contribute to the final statistical averages used to compute reflectance and other photometric properties. Implementing these boundary conditions also aids in conserving the total energy within the simulation domain. Photons that exit and re-enter the domain continue to interact with the medium, ensuring that the total energy accounted for in the simulation reflects the true behavior of a semi-infinite medium.

3.2.1 Defined Factors and Parameters:

- N = Number of photon packets to be simulated (10^4 in this case to reduce the computational time).
- rad = Radius of the particles in the medium (1 arbitrary unit).
- w = List of single scattering albedo values to simulate ($[0.7, 0.5, 0.2]$).
- Anisotropic scattering considered.
- i = Incidence angle of the incoming light (30deg).
- b = List of asymmetry factors ($[-0.5, 0, 0.5]$).
- ϕ = Volume fraction occupied by particles (0.2 in this case).
- $slab_depth$ = Depth of the slab medium (10 units).
- Semi-infinite medium with periodic boundary conditions.
- Henyey-Greenstein phase function used as single particle phase function.

Significant Factors:

- Reflectance $r(i, e, g)$: The ratio of the reflected light to the incident light for given incidence, emission, and phase angles.
- Single Scattering Albedo (SSA) w : The fraction of light scattered by a particle at each interaction. It is a critical parameter influencing the scattering and absorption processes within the medium.
- Single Scattering Phase Function $p(g)$: The probability density that light is scattered in a given direction at phase angle g . This function describes the angular distribution of scattered light and is essential for accurate photon path simulation. In this simulation, the Henyey-Greenstein phase function is used to determine the scattering angles of photons interacting with particles. This helps simulate realistic photon paths and energy distributions, essential for studying optical phenomena such as the Shadow Hiding Opposition Effect (SHOE) in a particulate medium.

The **Henyeey-Greenstein phase function** provides a simple analytical expression that can be easily implemented in simulations. It is given by: [Ciarniello et al., 2014]

$$p(g) = \frac{1 - b^2}{4\pi(1 + b^2 + 2b \cos(g))^{3/2}} \quad (3.3)$$

where g is the scattering angle, and b is the asymmetry parameter. This simplicity makes it computationally efficient. The parameter b in the Henyeey-Greenstein phase function allows for the adjustment of the asymmetry of the scattering.

- When $b = 0$, the phase function is isotropic, meaning the light is scattered equally in all directions.
- When $b > 0$, the function models forward scattering, which is common in many natural and engineered materials.
- When $b < 0$, the function models backward scattering.

3.2.2 Conditions Defined

Initial Photon Conditions:

- Photon packets start from the origin '(0, 0, 0)'.
- Initial direction of photons is determined by the incidence angle.
- Initial energy 'E₀' of photon packets is set to 1.0.
- Initial visibility 'h_i' of the photon is set to 1.

Boundary Conditions:

The medium is modeled as a finite box with horizontal dimensions determined by the number of particles and the filling factor. When photons escape from a lateral wall of the simulated box, they are reintroduced on the opposite side, conserving their propagation direction and depth. This process effectively mimics an infinite horizontal extension by ensuring that photons continue their paths without artificial boundaries.

Chapter 4

Results

In the initial phase of this project, I aimed to reproduce the plots from Ciarniello et al., 2014, for a slab characterized by the filling factor ϕ , which represents the volume fraction occupied by particles. The effect of ϕ on the simulated particulate medium was illustrated in Fig. 4.1.

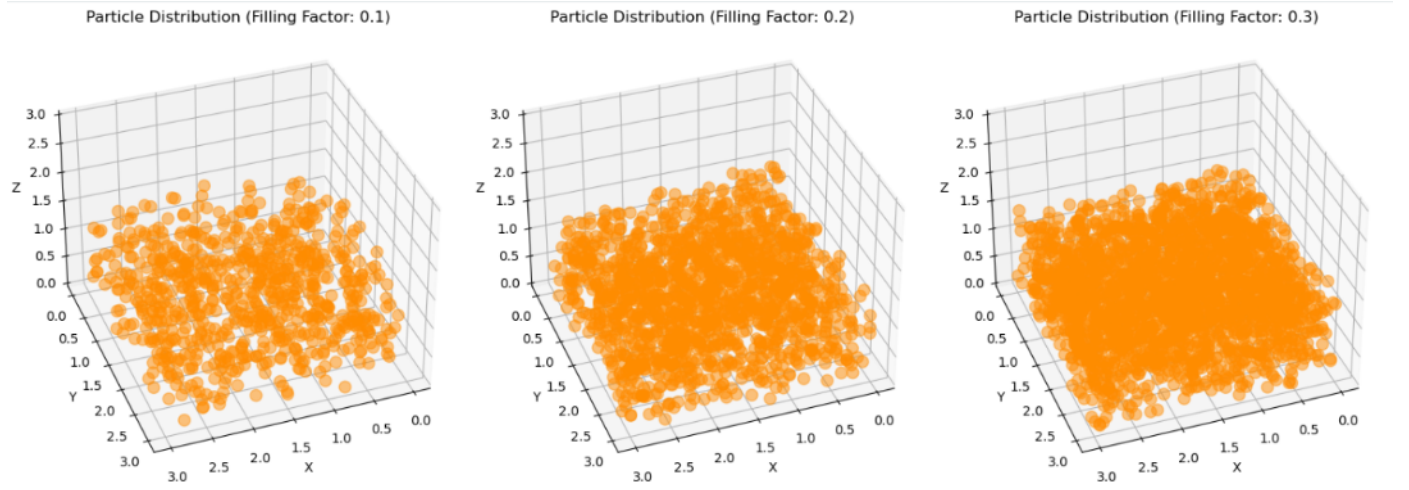


Figure 4.1: Volumes of simulated particulate media with different filling factor

In the Direct and Indirect MCRT methods, the consideration of the periodic boundary conditions plays a crucial role in accurately modeling radiative transfer. For photons propagated from the source, periodic boundaries ensure that photons continue their interactions with the medium regardless of their exit points from the domain. This is particularly important in high optical depth scenarios where multiple scattering events are significant. For photons traced backward from the observer, periodic boundaries ensure that potential paths leading back to the light source are correctly modeled. This approach captures the diffuse light transport effectively, accounting for all relevant scattering paths. By incorporating these characteristics and boundary conditions, MCRT simulations provide a robust and accurate representation of radiative transfer in a semi-infinite medium, ensuring that the simulated photometric properties are representative of real-world scenarios where the medium is effectively infinite or very large compared to the particle scale.

Following this, I simulated the Monte Carlo Radiative Transfer (MCRT) models using both direct and indirect methods, resulting in two separate plots. The description of the parameters and condi-

tions are discussed in Section 3.2. The plots can be altered to observe the effect of different variables and parameters.

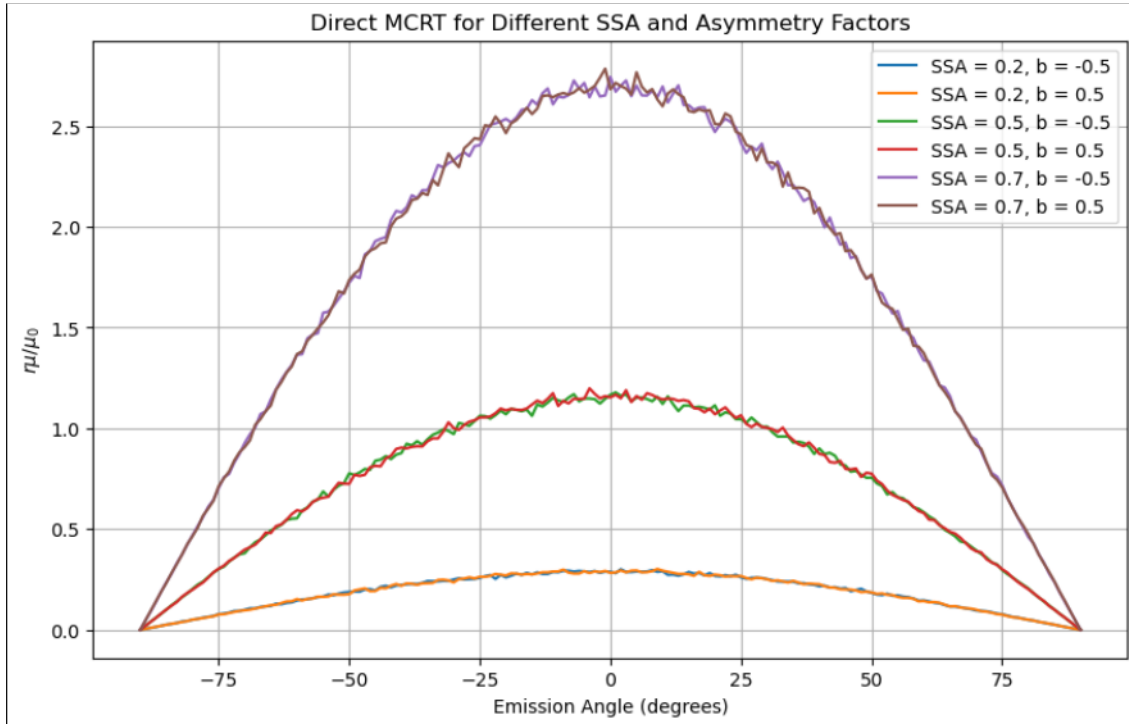


Figure 4.2: Plot obtained for the Direct MCRT simulation with parameters defined as in sec. 3.2.1

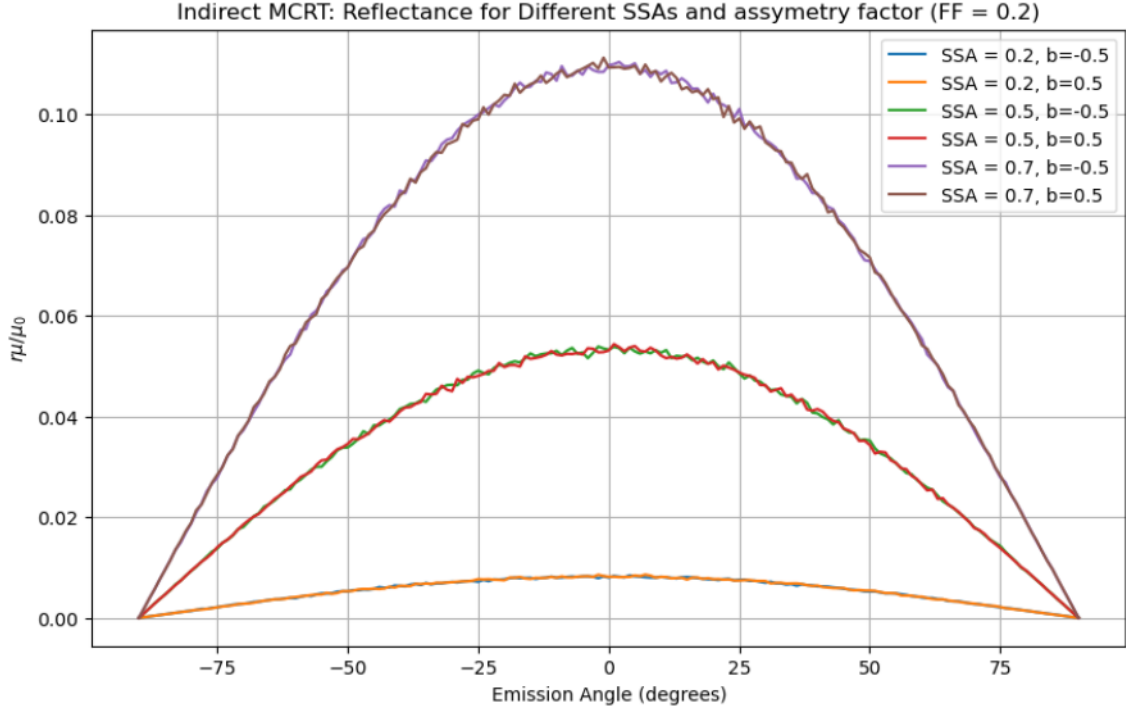


Figure 4.3: Plot obtained for the Indirect MCRT simulation with parameters defined as in sec. 3.2.1

However, several issues were encountered in the simulation results. Notably, the plots in fig. 4.2 and fig. 4.3 did not show any effect of the incidence angle or any peaks corresponding to the Shadow Hiding Opposition Effect (SHOE). This absence of expected features suggests that certain aspects of the model or its implementation needs further refinement.

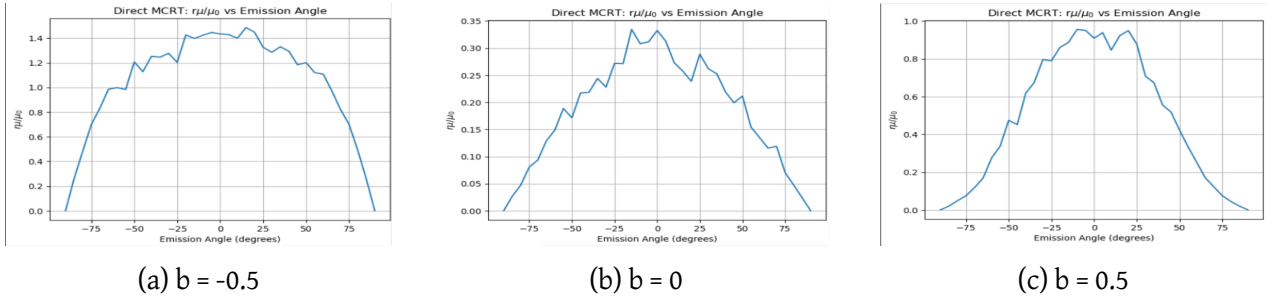


Figure 4.4: Trial plot to test anisotropy without boundary condition and reduced photon count

The Henyey-Greenstein function was employed to account for anisotropy and obtain the single particle phase function in all the plots shown. Despite varying the asymmetry parameter, there was no significant impact on the resulting plots, indicating potential issues with how the anisotropy is being modeled or applied in the simulation. However, in the initial trial steps of development, anisotropy effect could be slightly observed as shown in fig. 4.4 where boundary conditions was not taken into account. This suggests that the inconsistency might lie in the applications of boundary conditions in the medium.

Moreover, discrepancies were observed between the reflectance values obtained from the direct and indirect MCRT methods. This mismatch points to a possible issue with the normalization process in

the simulations which might be due to the consideration of lower number of photon packets which I did to reduce simulation time. This can be fixed if the above issues are resolved.

On a positive note, the effect of the filling factor(ϕ) and the SSA(w) on the shape of the reflectance curve was obtained as expected, demonstrating that some aspects of the model are functioning correctly.

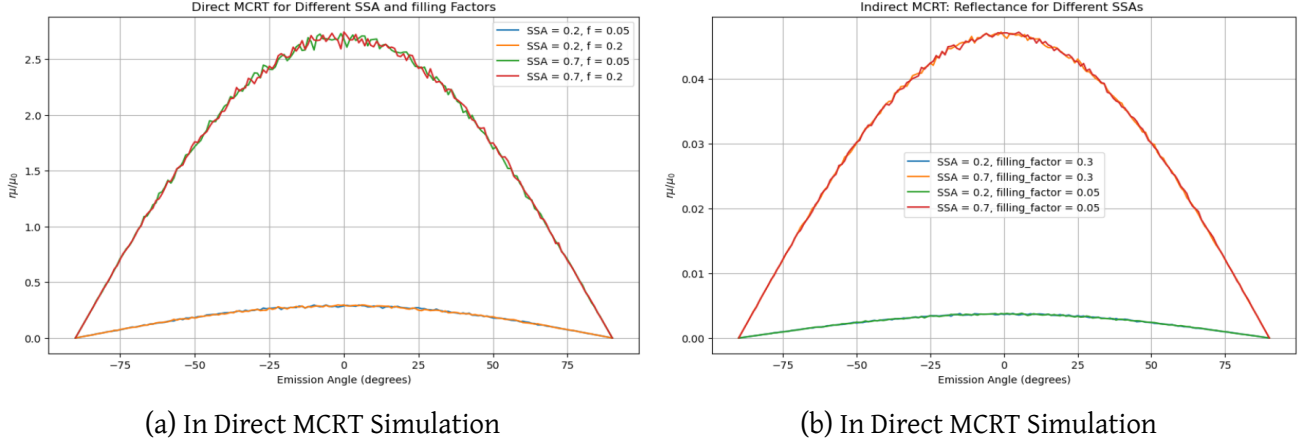


Figure 4.5: Plot on varying ϕ and SSA

4.1 Challenges

Several challenges were encountered during the development and implementation of the MCRT models:

- **Phase Function Calculation:** The phase function $p(g)$ seems to be not properly computed as a function of the phase angle at each scattering event with the correct b-value. This issue likely stems from not simulating a many-particle medium accurately, thus failing to capture the geometric effects of a discrete semi-infinite medium.
- **Photon Propagation Simulation:** The current code attempts to simulate a deep-enough slab of particles and follow the photon propagation geometrically from one particle to another. However, it treats the propagation length statistically, as if the medium were continuous. This approach may not fully capture the complexities of a particulate medium.
- **Boundary Conditions and Visibility Check:** There are potential issues with the periodic boundary conditions and the visibility check of scattered photons, which may contribute to the discrepancies observed between the direct and indirect methods.
- **Computational Time:** The extensive nature of the codes led to long simulation runtimes. This challenge is compounded by the need to balance accuracy and computational efficiency, especially given the project's time constraints.

4.2 Future prospects

This project could be improved if we focus on addressing the identified challenges and improving the accuracy and efficiency of the MCRT models. The computation of the phase function $p(g)$ can be refined to ensure it correctly accounts for the phase angle and b-value at each scattering event. A more accurate simulation of a many-particle medium has to be developed, possibly incorporating discrete particle interactions and geometric effects more effectively. The periodic boundary conditions and the visibility check mechanisms has to be revised to better capture the behavior of scattered photons in a semi-infinite medium. The plots from the reference Ciarniello et al., 2014 can be accurately reproduced on making appropriate modifications.

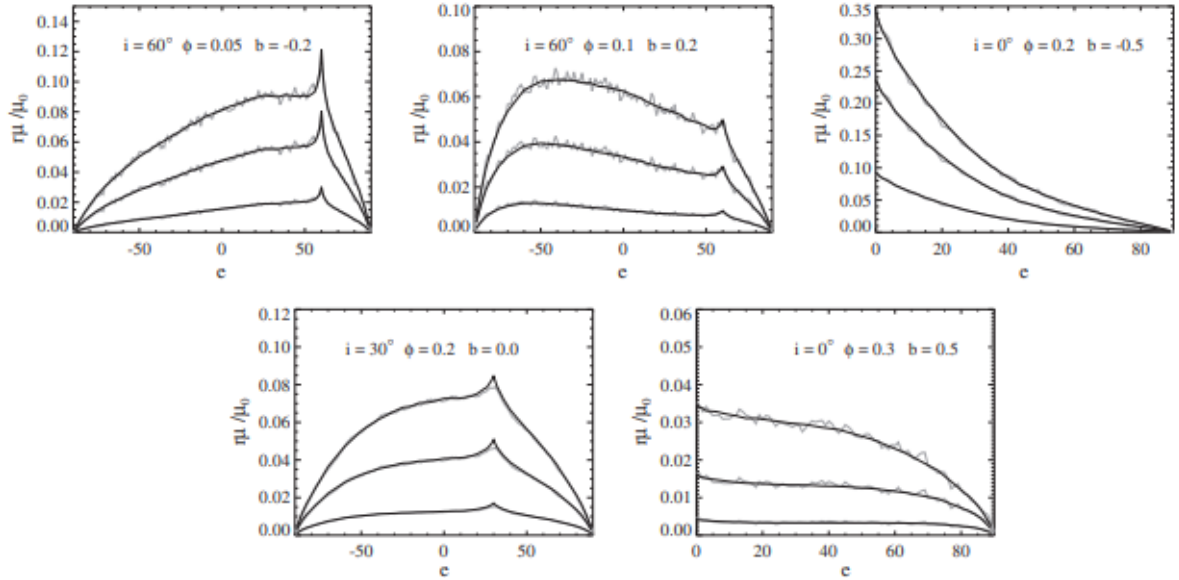


Figure 4.6: Expected plots as given in Ciarniello et al., 2014 to be obtained

Alternative computational methods or optimization techniques should be explored to reduce simulation runtime without compromising accuracy.

The ultimate goal of this project is to develop a robust tool for analyzing reflectance spectra from remote sensing data, such as those from the Chandrayaan mission. By comparing the MCRT results with the established Hapke model, we can gauge the accuracy of the MCRT approach and enhance our ability to derive physical properties from reflectance spectra. Continued efforts to improve the MCRT models will contribute significantly to the field of planetary science and the interpretation of remote sensing data.

Conclusion

In this summer project, I aimed to explore the Monte Carlo Radiative Transfer (MCRT) method for modeling the reflectance spectra of planetary surfaces, specifically to study the direct and indirect MCRT approaches. The primary objective of this project was to compare these methods to the established Hapke model and to analyze their potential for deriving physical properties from reflectance spectra obtained through remote sensing, such as those from the Chandrayaan mission.

Preliminary aim of the project sought to reproduce results from Ciarniello et al., 2014, focusing on the impact of the filling factor (ϕ) on the reflectance of a simulated particulate medium. These efforts were successful in some respects, with the effects of ϕ and single scattering albedo (SSA) on the reflectance curve being consistent with expectations. However, challenges emerged in capturing the effects of the incidence angle and the Shadow Hiding Opposition Effect (SHOE), which are critical for accurately modeling planetary surfaces.

The Henyey-Greenstein phase function was employed to account for anisotropy, yet variations in the asymmetry parameter did not yield significant changes in the reflectance plots. This suggests potential issues in the implementation of anisotropic scattering in the model or the periodic boundary conditions. Furthermore, discrepancies between the reflectance values from the direct and indirect MCRT methods pointed to possible normalization issues, highlighting the need for further refinement.

The primary challenges encountered included inaccuracies in the phase function calculation, difficulties in simulating a many-particle medium, and issues with periodic boundary conditions and visibility checks for scattered photons. These factors contributed to the inability to fully capture the geometric effects of a discrete semi-infinite medium, which is crucial for realistic reflectance modeling. Despite these challenges, the project demonstrated that the MCRT method holds promise for modeling reflectance spectra. The next steps involve addressing the identified issues, particularly improving phase function accuracy, enhancing medium simulation, and optimizing boundary conditions. Additionally, reducing computational time through alternative methods or optimization techniques is essential for practical application.

In conclusion, this project has laid the groundwork for utilizing the MCRT method in planetary reflectance studies. While further work is needed to resolve current challenges and improve model accuracy, the potential for this method to complement and enhance traditional models like Hapke's is evident. Successful refinement of the MCRT approach will provide a valuable tool for analyzing remote sensing data, enabling more accurate derivation of physical properties from planetary reflectance spectra. This advancement will significantly contribute to our understanding of planetary surfaces and the interpretation of data from various planetary missions.

Nomenclature

Abbreviations

AMSA	Anisotropic Multiple Scattering
BDR	Bi-Directional Reflectance
BRDF	Bidirectional Reflectance Distribution Function
CBOE	Coherent Backscattering Opposition Effect
H2008	Hapke 2008
IMSA	Isotropic Multiple Scattering
MCRT	Monte Carlo Radiative Transfer
SHOE	Shadow Hiding Opposition effect
SSA	Single Scattering Albedo

Symbols

μ_e	Effective cosine of the emission angle
μ_{0e}	Effective cosine of the incidence angle
ϕ	Filling factor, the fraction of the volume occupied by particles
τ	Optical Depth of the slab medium.
b	Asymmetry factor for the Henyey-Greenstein phase function.
B_{CB}	Coherent backscatter opposition effect
B_{SH}	Shadow hiding opposition effect
c	Empirical parameters determining the shape and strength of scattering lobes
e	Emission angle of scattered photons (in degrees).
E_0	The initial energy of the photon packet
g	Phase angle

h_i	Visibility parameter
i	Incidence angle of incoming photons (in degrees).
K	Porosity correction factor
$M(\mu_{0e}/K, \mu_e/K, g)$	Multiple scattering
N	Number of photon packets to simulate.
$p(g_i)$	The single scattering phase function at the phase angle g_i
$S(\mu_{0e}, \mu_e, \psi)$	Shadowing on rough surfaces, depending on the azimuth angle ψ
w	Single scattering albedo
rad	Radius of particles in the medium.

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Appendices

Appendix A

Codes

Listing A.1: Python code to simulate the effect of ϕ on the particulate medium volume

```
# Define the slab properties
slab_width = 3
slab_height = 3
slab_depth = 1.5

# Define the particle properties
particle_radius = 0.08

# Define the range of filling factors
phi_s = [0.1, 0.2, 0.3]

# Number of rays for the simulation
num_rays = 10e4

def gen_particle(slab_dim, w):
    volume_slab = slab_dim[0] * slab_dim[1] * slab_dim[2]
    volume_particle = (4/3) * np.pi * particle_radius**3
    n_part = int(w * volume_slab / volume_particle)

    particles = np.random.uniform(0, slab_dim, (n_part, 3))
    return particles

def monte_carlo_ray_tracing(slab_dim, particles, num_rays):
    reflectance = 0
    for _ in tqdm(range(num_rays), desc="Simulating rays"):
        # Generate a ray entering the slab
        ray_origin = np.random.uniform(0, slab_dim[0]),
            np.random.uniform(0, slab_dim[1]), 0
        ray_direction = np.array([0, 0, 1])
```

```

        while ray_origin[2] < slab_dim[2]:
            distances = np.linalg.norm(particles - ray_origin, axis=1)
            if np.any(distances <= particle_radius):
                reflectance += 1
                break
            ray_origin = ray_origin + ray_direction * 1

    return reflectance / num_rays

# 3D plot function to visualize particle distribution
def plot_particle_distribution(ax, particles, phi):
    ax.scatter(particles[:, 0], particles[:, 1], particles[:, 2],
               c='darkorange', marker='o', s=80, alpha=0.5)
    ax.set_zlim(0, 3)
    ax.set_xlabel('X')
    ax.set_ylabel('Y')
    ax.set_zlabel('Z')
    ax.set_title(f'Particle Distribution (Filling Factor: {phi})')
    ax.view_init(elev=35, azim=70)

# Simulate for different filling factors
fig = plt.figure(figsize=(12, 9))

for i, phi in enumerate(phi_s):
    # Generate particles
    particles = gen_particle((slab_width, slab_height, slab_depth), phi)
    # Plot particle distribution
    ax = fig.add_subplot(2, 3, i+1, projection='3d')
    plot_particle_distribution(ax, particles, phi)

plt.tight_layout()
plt.show()

```

Listing A.2: Python code to simulate the Direct MCRT Method with the implementation of appropriate periodic Boundary Conditions for different SSA and b

```

# DIRECT MCRT

def HG_phase_function(g, b):
    """Henyey-Greenstein phase function."""
    return (1-b**2)/(4*np.pi*(1 + b**2 + 2*b*np.cos(g))**(3/2))

def compute_slab_depth(phi, radius):

```

```

cross_sectional_area = np.pi * radius**2
mean_free_path = 1 / (phi * cross_sectional_area)
# Set the slab depth to be several times the mean free path
slab_depth = (10**6) * mean_free_path
return slab_depth

def direct_mcrt(n_photons, radius, ssa, i_ang, b, f):
    slab_depth = compute_slab_depth(f, radius)
    r_mu_over_mu_0 = []
    mu_0 = np.cos(np.radians(i_ang))

    for emission_angle in tqdm(range(-90, 91, 1)):
        # Emission angle range from -90 to 90 degrees
        photons_scattered = 0
        mu = np.cos(np.radians(emission_angle))

        for _ in range(n_photons):
            x, y, z = 0, 0, 0 # Starting at the origin

            # Initial photon direction based on incidence angle
            direction = np.array([np.sin(np.radians(i_ang)),
                                  0,
                                  np.cos(np.radians(i_ang))])

            while True:
                # Absorption Probability
                v1 = np.random.rand()
                if v1 > ssa:
                    break # Photon absorbed

                # To determine the scattering angle
                while True:
                    g_guess = np.random.uniform(0, np.pi)
                    # Guess for scattering angle
                    p_g_guess = HG_phase_function(g_guess, b)
                    dP_dg = p_g_guess * 2 * np.pi * np.sin(g_guess)
                    # PDF for scattering at angle g_guess

                    v2 = np.random.rand() * dP_dg.max()
                    # Random variable uniformly distributed
                    from 0 to max_dP_dg
                    if dP_dg > v2:
                        g = g_guess
                        # Accept g_guess as scattering angle

```

break

```
# Azimuthal Angle Determination
psi = 2 * np.pi * np.random.rand()
# Azimuthal angle uniformly distributed from 0 to 2pi

# Update photon direction using scattering angles
direction[0] = np.sin(g) * np.cos(psi)
direction[1] = np.sin(g) * np.sin(psi)
direction[2] = np.cos(g)

# Update photon position
x += direction[0]
y += direction[1]
z += direction[2]

# Apply periodic boundary conditions
x = x % (2 * radius)
y = y % (2 * radius)
z = z % (2 * radius)

# Escape condition:
# ensure photons do not exceed slab depth
if z > slab_depth:
    break # Photon escaped

# Increase count of scattered photons
photons_scattered += 1

reflectance = photons_scattered / n_photons
r_mu_over_mu_0.append(reflectance * mu / mu_0)
```

return r_mu_over_mu_0

```
# Simulation parameters
n_photons = 10**4
# Reduced number of photons for faster computation
radius = 0.01 # Arbitrary unit
ssas = [0.2, 0.5, 0.7]
# Assumed single scattering albedos
i_ang = 30 # Incidence angle in degrees
bs = [-0.5, 0.5] # Asymmetry factors
f = 0.2 # Filling factor
```

```

# Plot results for each asymmetry factor and SSA
plt.figure(figsize=(10, 6))
for ssa in ssas:
    for b in bs:
        # Run direct MCRT simulation
        r_mu_over_mu_0 = direct_mcrt(n_photons, radius, ssa,
                                      i_ang, b, f)

        # Plot results
        e_ang = np.arange(-90, 91, 1)
        plt.plot(e_ang, r_mu_over_mu_0, label=f'SSA = {ssa}, b = {b}')

plt.xlabel('Emission Angle (degrees)')
plt.ylabel(r'$r\mu / \mu_0$')
plt.title('Direct MCRT for Different SSA and Asymmetry Factors')
plt.grid(True)
plt.legend()
plt.show()

```

Listing A.3: Python code to simulate the Indirect MCRT Method with the implementation of periodic Boundary Conditions

```

# INDIRECT MCRT

def HG_phase_function(g, b):
    """Henyey-Greenstein phase function."""
    return (1-b**2)/(4*np.pi*(1+b**2+2*b*np.cos(g))**(3/2))

def compute_slab_depth(phi, radius):
    cross_sectional_area = np.pi * radius**2
    mean_free_path = 1 / (phi * cross_sectional_area)
    # Set the slab depth to be several times the mean free path
    slab_depth = 10**6 * mean_free_path
    return slab_depth

def indirect_mcrt(n_photons, radius, ssa, i_ang, b, phi):
    slab_depth = compute_slab_depth(phi, radius)
    r_mu_over_mu_0 = []
    mu_0 = np.cos(np.radians(i_ang))
    E_0 = 1.0 # Initial energy of the photon packet

    for emission_angle in tqdm(range(-90, 91, 1)):
        # Emission angle range from -90 to 90 degrees
        total_energy = 0.0

```



```

mu = np.cos(np.radians(emission_angle))

for _ in range(n_photons):
    # Start photon at the surface of the particle
    theta = np.random.rand() * 2 * np.pi
    x, y, z = radius * np.cos(theta),
               radius * np.sin(theta), 0
    # Initial photon direction based on incidence angle
    direction = np.array([np.sin(np.radians(i_ang)), 0,
                          np.cos(np.radians(i_ang))])

    energy = E_0
    # Initial energy of the photon packet
    h_i = 1
    # Initial visibility of the photon

    while energy > 0.001:
        # Continue until the energy is negligible
        # Distance to next scattering event
        mean_free_path = 1 / (phi * np.pi * radius**2)
        travel_distance = -mean_free_path *
                          np.log(np.random.rand())

        # Update photon position
        x += travel_distance * direction[0]
        y += travel_distance * direction[1]
        z += travel_distance * direction[2]

        # Apply periodic boundary conditions
        x = x % (2 * radius)
        y = y % (2 * radius)
        z = z % (2 * radius)

        # Check if the photon escapes
        if z > slab_depth:
            break

        # Absorption Probability
        if np.random.rand() > ssa:
            break # Photon absorbed

        # Scattering Angle Determination
        while True:
            g_guess = np.random.uniform(0, np.pi)

```

```

        # Guess for scattering angle
        p_g_guess = HG_phase_function(g_guess, b)
        dP_dg = p_g_guess * 2 * np.pi * np.sin(g_guess)
        if np.random.rand() < dP_dg:
            g = g_guess
            # Accept g_guess as scattering angle
            break

    # Azimuthal Angle Determination
    psi = 2 * np.pi * np.random.rand()
    # Azimuthal angle uniformly distributed from 0 to 2pi

    # Update photon direction using scattering angles
    direction[0] = np.sin(g) * np.cos(psi)
    direction[1] = np.sin(g) * np.sin(psi)
    direction[2] = np.cos(g)

    # Energy reduction after scattering
    energy *= ssa * HG_phase_function(g, b)

    total_energy += energy

    reflectance = total_energy / (n_photons * E_0)
    r_mu_over_mu_0.append(reflectance * mu / mu_0)

    return r_mu_over_mu_0

# Simulation parameters
n_photons = 2*(10**4) # Number of photons
radius = 0.01 # Arbitrary unit
ssas = [0.2, 0.5, 0.7] # Different SSAs
i_ang = 30 # Incidence angle in degrees
b = [-0.5, 0.5] # Asymmetry factor
phi = 0.2 # Fixed filling factor

# Run indirect MCRT simulation
# for different SSAs and assymetry factor

plt.figure(figsize=(10, 6))
for ssa in ssas:
    for b in bs:
        r_mu_over_mu_0 = indirect_mcrt(n_photons, radius, ssa, i_ang,
        b, phi)

```

```

# Plot results
e_ang = np.arange(-90, 91, 1)
plt.plot(e_ang, r_mu_over_mu_0,
label=f'SSA = {ssa}, b={b}')

plt.xlabel('Emission Angle (degrees)')
plt.ylabel(r'$r\mu / \mu_0$')
plt.title(r'Indirect MCRT: Reflectance for Different SSAs and
assymetry factor ($\phi = 0.2$)')
plt.legend()
plt.grid(True)
plt.show()

```