A Condensed History Model for Photon-Electron Transport in Binary Markovian-Mixed Media

by

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A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy (Nuclear Engineering and Radiological Sciences) in The University of Michigan 2023

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This material is based upon work supported by the Department of Energy Nuclear Energy University Programs Graduate Fellowship and Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.
ACKNOWLEDGEMENTS

Thank you to my advisor Dr. Brian Kiedrowski for the opportunity to pursue a doctorate degree. Thank you to my committee members, Dr. Edward Larsen, Dr. Scott Baalrud, and Dr. Stilian Stoev for serving on my committee. Thank you Dr. Aaron Olson at Sandia National Laboratories and Dr. Patrick Brantley at Lawrence Livermore National Laboratory for mentoring me during my time at each institution and providing me opportunities to publish and grow as an independent researcher early in my graduate career. My professional career and life are a palimpsest of my experience at the labs. Thank you to Shannon Thomas for all of your help in managing my research funding.

Completing this program would not have been possible without the love and support of so many people. I owe the biggest thank you and appreciation to my mom and dad for their many sacrifices that have allowed me to continue following my dreams, for their undying support and encouragement, and for their unconditional love that reminds me of how lucky I am to have them as my parents. I am so lucky to have my brothers Michael and Victor, whom I always look forward to seeing when I am able to come home for the holidays. Thank you for traveling a great distance to attend my defense in-person on November 28, 2022.

I would like to thank my chosen family. Thank you for supporting me and for keeping in touch with me after all these years. Thank you to my elementary school friends Jilly Dos Santos, Maddy Mueller, and Bailey Washer. Thank you to Jessica Chow, Jason Coffman, and Marina Fox from UC Berkeley. Thank you to Talia and Javi Martinez, who made my summers in Albuquerque a blast. Thank you to my newest friends Kara Steshetz, Christa Hansma, Eileen Li, Christina Brietzke, Rawan Najar, Hollis Cuffie, Robin Johnson, and
Ariana Biddle for making my day-to-day throughout this program bearable. Thank you to Chelsea Duong for the year of 2019, a year full of tomfoolery and a gold standard for my years to come (see Spotify code in Figure 0.1).

Thank you to the members of my academic geneology, Aaron Tumulak, Evan Gonzalez, Kyle Beyer, and Eric Pearson. Thank you Aaron Tumulak, especially. I owe you a few more pints of ice cream. Thank you to Avery Grieve for their MCNP support. Thank you Dr. Rachel Slaybaugh at UC Berkeley for providing me many opportunities during my undergraduate career that prepared me for graduate school. Thank you to the graduate students of the Nuclear Engineering Department at UC Berkeley, Marissa Ramirez de Chanlatte, Milos Atz, James Kendrick, Chris Poresky, Mario Ortega, Jessica Rehak, Alex Droster, Mitch Negus, Sami Lewis, and Vanessa Goss as well as honorary graduate students Samuel Varghese and Laura Shi for positively impacting my undergraduate experience. Thank you to Dr. Carolyn Kuranz and Dr. John Foster for being invaluable resources to me. Additionally, thank you to the women at this university, Dr. Carolyn Kuranz, Dr. Laura Hirshfield, Roxanne Walker, Leah Clark, Jenny Smith, Stephanie Miller, Sara Bashir, and Mackenzie Warwick for all of your wisdom, support, and words of encouragement. Thank you also to Dr. Dixie Hu for all that you have done.

Thank you to Delta Nu members Anna Morgan, Melanie Chausseur, Natalie Baughan, and Corbin Bennett, for giving me a taste of that sweet sisterhood bond. Thank you to the Mallon Family, who I consider family, for welcoming me into your home and for being a part of many of my graduate school memories. And to Emma Mallon, my partner in crime who I love and adore from the bottom of my heart, thank you for being my biggest supporter and for all of the memories we made along the way. We can finally bask in the sun.

Last but certainly not least, thank you to my strong band of Instagram followers and fans who have kept up with my story and supported me from afar.
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ABSTRACT

This dissertation presents a novel condensed history method applicable to photon-electron transport problems in which the background materials are not precisely known but prescribed by random spatial mixing distributions. This method accurately incorporates the underlying randomness of the background materials and is significantly more efficient than current approaches that require simulating particle transport on numerous fully generated random realizations, effectively extending the range of problems that can be practically analyzed. Generalized multi-scatter distributions are derived to account for multiple materials within a stochastic region on an on-average basis such that material geometries do not have to be fully generated to simulate an electron track. The capabilities of this model are demonstrated by investigating beam source problems on single-region and multi-region slab geometries of binary, Markovian mixtures and computing mean particle leakage rates and electron energy deposition for both electron source and photon source problems. A novel capability of computing material-dependent energy deposition by the electron is demonstrated. The accuracy of this model for photon-electron transport is evaluated by comparing its results against benchmark results obtained using a single-scatter and condensed history Monte Carlo approach on fully generated material realizations. This work finds that, for the single-region slab problems investigated, this new condensed history model generally produced electron leakage rates with roughly a mean absolute relative error of 8-19% and 5-10% when compared against single-scatter and condensed history benchmark results, respectively. For multi-region slab problems investigated, this new condensed history model generally produced electron leakage rates with roughly a mean absolute relative error of 15% and 28% when compared against single-scatter and condensed history benchmark results, respectively.
For material-dependent electron energy deposition results, the mean absolute relative error achieved was within about 15% for single-region slab problems and within about 30% for multi-region slab problems compared to condensed history benchmark results.
CHAPTER 1

Introduction

This dissertation develops a photon-electron transport condensed history method that is applicable to binary stochastic media. This chapter begins by motivating the research topic in Section 1.1 and identifies gaps and challenges in this area of particle transport. This chapter then gives a broad overview of numerical methods used to model particle transport in Section 1.2. A summary of established work done in Monte Carlo methods for electron transport as well as in transport in stochastic media are then provided in Section 1.3 and Section 1.4, respectively. A review of current work that aims to address electron transport in stochastic media is then provided in Section 1.5. Finally, Section 1.6 gives the outline of the remainder of this dissertation.

1.1 Motivation of Work

The ability to accurately and efficiently model the transport of high-energy electrons (> 1 keV) through matter is vital for many applications because as an electron moves through matter, it can interact with the background materials and deposit its kinetic energy. This is especially important in applications such as in radiation oncology, where potentially cancerous organ tissue undergoes diagnostics and radiation treatment. During this treatment, high energy electrons can be produced and interact with the host tissue. A common concern when undergoing these treatments is the dose of radiation received by surrounding healthy
Another application is accurately computing the detailed energy balance in inertial confinement fusion (ICF) problems. In inertial fusion, a capsule containing fusion fuel is rapidly compressed by lasers and is turned into plasma. While fusion occurs, fast electrons are produced from gamma and x-ray interactions and transport energy as they move through the system. Another application of interest is in radiation hardening. Electronic components employed in outer-space are exposed to highly ionizing radiation fields and may be damaged by the energy deposited by electrons. For these components to become more resistant to the heating and damage caused by high energy electrons in this environment, they must be “hardened.”

Providing capability for analyzing high-energy electron transport supports research in a plethora of fields. To model electron transport, it usually must be coupled with photon transport because secondary electrons are produced in photon collisions, and the slowing down of those electrons produces more photons. Monte Carlo methods are routinely used by engineers and medical physicists to infer characteristics of a photon-electron field from numerous sampled particle trajectories. The quantum mechanical nature of particle interactions make this process inherently random, and the probability distributions for individual photon and electron interactions and how to model these interactions using a Monte Carlo approach are known.

However, an arduous challenge associated with using a Monte Carlo approach to model a photon-electron field is the extensive computational runtime required to achieve a resolved result because of the large number of interactions an electron may experience. Electrons arising from ionization or nuclear processes typically experience an order of $10^5$ interactions within the span of a few millimeters, which may result in the compounding emission of secondary particles. Therefore, conducting a detailed simulation of this random process is usually impractical and often unnecessary for routine engineering design calculations.

To address this challenge, the condensed history method was developed and is used in many current Monte Carlo codes. This Monte Carlo algorithm samples probability distribu-
tions describing numerous electron interactions, as opposed to the probability distributions used in a detailed Monte Carlo approach describing single electron interactions. Though the condensed history method significantly improves the computational runtime of photon-electron transport problems, the method only applies to problems with a uniform background material. This is because homogeneous background materials the probability distributions currently sampled in a condensed history method were derived assuming a homogeneous background materials.

In many applications, however, the background material properties are non-uniform and have random spatial variation governed by material mixing statistics or probabilities. In these stochastic material mixtures, an individual particle will travel through a random number of randomly oriented regions containing different (also random) material types that are not accounted for in the probability distributions currently used in condensed history algorithms. Therefore, of the approaches currently available, the computationally expensive “brute force” approach of simulating each individual electron interaction on numerous random material mixtures is required for these types of problems. Some examples of applications with stochastic material mixing are:

- material mixing because of Rayleigh-Taylor instabilities that occur in ICF problems [31],
- organ tissue that may undergo tissue diagnostics and optics in the medical physics field [96],
- fuel kernels used in pebble bed reactors [52, 73, 110],
- engineered optical materials used for light propagation [90, 91, 104],
- clouds when conducting climate studies in the meteorology field [46, 59, 111].

This dissertation attempts to address the limitations of the condensed history algorithm and extend its range of applicability to stochastic material mixing problems. This work develops a statistical condensed history model and simulation method that adequately accounts
for the underlying randomness of the material properties given some prescribed distribution function while preserving as much physics from the individual electron interactions as feasible and while maintaining computational performance. The analysis in this dissertation is restricted to binary, Markovian mixtures.

1.2 Numerical Methods for Particle Transport

This section provides a general survey of two major classes of numerical methods used for particle transport: deterministic and Monte Carlo. In addition to providing a broad background of these two approaches, this section demonstrates how the current dissertation project compares and contrasts with the numerous approaches currently available for modeling the transport of radiation through matter.

1.2.1 Deterministic Approach

The deterministic approach approximates the governing transport equation by discretizing the phase space and/or expanding the solution in terms of a set of basis functions. A large majority of electron scatters are highly forward-peaked and result in small energy changes (soft collisions). Electrons infrequently experience a collision that results in a large energy loss and direction change (hard collisions). Because of the many highly forward-peaked scatters an electron experiences, a large number of expansion terms would be required to accurately capture the scattering behavior, making it rather difficult to compute. Because of this, the continuous-slowing down approximation (CSDA) is often made before applying a deterministic solver, yielding the Fokker-Planck equation [74]. Further approximations may also be made to yield the Boltzmann-Fokker-Planck equation [16, 72], in which the electron collision term is separated between soft and hard collisions. The soft collision term of the electron is approximated with the CSDA, and the hard collision term of the electron is expanded requiring less terms.

The method of spherical harmonics (or $P_N$ method) is one deterministic scheme, which
expands the solution in terms of the spherical harmonic functions to create a coupled system of integro-differential equations for the expansion coefficients. The spatial and energy variables are then discretized to form an approximate linear system that may then be solved using numerical linear algebra schemes. An example of a code that uses the spherical harmonics $P_N$ method is Sandia Computational Engineer for Particle Transport for Radiation Effects (SCEPTRE) [15], a production code developed by Sandia National Laboratories (SNL).

The method of discrete ordinates (or $S_N$ method) is perhaps the most common deterministic scheme, which discretizes the directional and spatial variables. The directional variable of the particle field is a set of discrete directions (ordinates) based on a numerical quadrature set chosen to preserve angularly-integrated properties of the solution. A system of first-order differential equations in space is formed using this quadrature set and is coupled by the scattering process. This coupled system of equations is then spatially discretized to create a very large approximate linear system that must be solved using iterative techniques in a way that minimizes the required computer memory. The discrete ordinates $S_N$ method is also used in SCEPTRE as well as in ONELD, which is a code developed by Los Alamos National Laboratory (LANL) that models the electron-photon cascade [58].

Though using a deterministic approach is generally more computationally efficient than using a Monte Carlo approach, many of the spatial discretization schemes in the $P_N$ and $S_N$ methods often lead to non-physical negative solutions, which interferes with the solution method. These usually necessitate a “fix-up” scheme. In 2-D or 3-D problems, the discretization of the direction variable in the $S_N$ method leads to numerical oscillations called ray effects that negatively impact the quality of the solution. These are difficult to eliminate entirely in practice because both the spatial and directional discretizations would need to be refined to an impractical degree. In some applications with more complex geometries, it may also be difficult and impractical to model a radiation field using a deterministic approach because surfaces can not be exactly represented using spatial discretization. Additionally, unlike neutral particles, which often experience infrequent large changes in direction over large
distances traveled, electrons have significantly smaller mean free paths and typically undergo frequent, small changes in direction, requiring finer spatial and angular discretization, which poses computational and memory challenges when using a deterministic approach.

1.2.2 Monte Carlo Approach

The Monte Carlo approach samples from probability distributions to simulate the underlying random physical process of particle transport, which allows for this approach to be used on problems with complex geometries. Integral quantities are estimated from the mean behavior of the simulated particle trajectories. Monte Carlo calculations simulate the entire particle history, which includes secondary particles produced during a history and each individual interaction a particle may experience during its lifetime until its termination. In theory, when no other approximations are made within the method (cf. the condensed history method), Monte Carlo calculations converge to an exact result when simulating an infinite number of histories. This method lends well to producing accurate results for problems with complex geometries that otherwise would be intractable to solve using deterministic schemes. Unlike deterministic schemes, its accuracy is not limited by the approximations introduced by discretization and truncation of basis expansions. The Monte Carlo approach also retains directional dependence of scattering, which is advantageous for electron transport where scattering is very forward-peaked.

The major drawback of the Monte Carlo method is that the estimates of integral quantities are often slow to converge compared to the deterministic approach. The statistical nature of the method implies that its convergence rate is inversely proportional to the square root of the number of particle histories, which is a consequence of the central limit theorem from probability theory. The computational costs are further compounded for electron transport (either single scatter or condensed history) versus neutral particles because of the mean number of interactions, which greatly increases the computational time per history.
1.3 Monte Carlo Electron Transport Methods

This section provides an overview of Monte Carlo approaches that have been developed for electron transport. The accurate but computationally expensive single-scatter Monte Carlo approach is discussed as well as the different classes of condensed history algorithms. In addition, this section discusses common multi-scatter theories used in current condensed history algorithms as well as a summary of the history of production Monte Carlo electron transport codes.

Monte Carlo simulations can be used in an analog (single-scatter) manner to model the individual interactions of an electron history. These interactions include elastic scattering, inelastic scattering, bremsstrahlung emission, and positron annihilation. However, utilizing a single-scatter Monte Carlo approach for high-energy electron transport simulations is computationally expensive because of the $10^5 - 10^6$ of interactions that may occur as the kinetic energy of an electron reduces from around 1 MeV (a typical starting energy for a free electron or positron produced by Compton scattering or pair production) to 1 keV [40, 109].

A more efficient approach employs multi-scatter distributions that describe the transport of the electron over many interactions by assuming that the path of the electron is a straight trajectory. Sampling these distributions instead allows, in principle, for a Monte Carlo simulation to describe the same energy-loss physics using fewer operations. However, for low-energy electrons (< 1 keV), single-scatter simulations are necessary because a straight trajectory can no longer be assumed, decreasing the accuracy of these multi-scatter distributions [4].

1.3.1 Angular Deflection

The first multi-scatter distribution for angular deflection was developed by Molière, which assumes small scattering angles and an infinite medium. The distribution does not preserve the physics of single-scatter events and requires that at least 20 collisions are represented within a substep length [61]. The distribution lacks accuracy for low energy electrons and
Goudsmit and Saunderson developed a more robust theory for multi-scatter angular
deflection distributions using a Legendre polynomial expansion [30]. This distribution pre-
serves single-scatter physics and is commonly used in standard Monte Carlo codes for coupled
electron-photon transport such as in Electron TRANsport (ETRAN), Integrated Tiger Se-
ries (ITS), and Monte Carlo N-Particle (MCNP).

The theory is also consistent with an expression later introduced by Lewis. Lewis derived
a multi-scatter angular deflection distribution using spherical harmonics to obtain exact re-
sults rather than a small-angle approximation [56] as well as spatial moments that are often
used in deterministic electron transport codes. The coefficients derived from the higher
moments of the spatial distribution were shown to agree with the results of Goudsmit and
Saunderson.

1.3.2 Energy Loss Straggling

The mean energy loss of an electron can be described by its stopping power, which is
dependent on the electron energy the medium it is traversing. However, the energy loss of
electrons exhibit broad statistical fluctuations. These large statistical fluctuations must be
considered to accurately describe the electron field. Landau established a multi-scatter en-
ergy loss straggling distribution, which was derived such that the energy loss of the electron
is small compared to its initial energy [47].

However, error is introduced from the truncation of a Taylor series expansion in the
derivation. Williams later showed that the Landau distribution is not sufficiently accurate
to describe experimental results obtained by White and Millington [106]. The reason is that
the half-width of the Landau distribution is too small, and Williams identified that a Gaus-
sian distribution is a more accurate description of the physics [107]. Blunck and Leisegang
improved the accuracy of this distribution by convolving Landau's energy loss straggling
distribution with a Gaussian and defining the variance of the Gaussian by preserving the
second moment to yield a wider peak [7].

Chechin and Ermilova [17] conducted an error analysis that showed the improvements to Landau’s distribution by Blunck and Leisgang including a second order term are minor. However, this led to the estimation of an error term that was subsequently used by Seltzer [85] to refine the convolved distribution with an improved variance. This form of the energy-loss straggling distribution is employed in current generations of codes including Electron Transport (ETRAN) [83], Integrated TIGER Series (ITS) [53], and Monte Carlo N-Particle (MCNP) [109].

1.3.3 Condensed History Algorithms

Utilizing these multi-scatter theories in a condensed history random walk model allows for a significant improvement in runtime compared to a single-scatter electron Monte Carlo simulation while introducing some spatial discretization errors into the solution. Notably, there exists two variations of a condensed random walk developed [5], the first (Class I) being simpler but less accurate than the second (Class II).

The Class I algorithms define a step length that an electron traverses throughout its random walk based on a set energy loss. Typically, an energy loss of 8.3% is used because of the optimal trade-off between accuracy (from using small step lengths) and runtime (from having fewer computing operations as a result of using larger step lengths). At each step and substep, multi-scatter distributions are used to sample a new, cumulative energy loss and direction of flight, respectively. At the end of each substep, the production of secondary particles is handled in an analog manner such that the algorithm does not distinguish between collisions that result in small direction change and energy loss fraction (soft collisions) and collisions that result in both a large direction change and energy loss fraction (hard collisions) as well as the production of a secondary particle (catastrophic events). The Class I condensed history algorithm is commonly used in current Monte Carlo codes for coupled electron-photon transport such as in Electron TRANsport (ETRAN), Integrated Tiger Se-
ries (ITS), and Monte Carlo N-Particle (MCNP).

The Class II algorithm determines the electron path based on the event of a hard collision such that each pathlength traveled assumes a continuous-slowing-down process and ends with a catastrophic event in which the particle loses a large energy fraction and produces a secondary particle. Compared to Class I, the Class II algorithm is more computationally demanding but more accurately preserves the correlation between multiple scattering deflections and energy loss fluctuations. It more concretely initializes secondary particles produced, and more accurately computes the angular deflection due to inelastic scatters. The random-hinge method [28] is a notable implementation of the Class II condensed history scheme. This method condenses an electron history by simulating the probabilistic overall effect of soft collisions between hard collisions and then randomly sampling the segment between two hard collisions at which the electron trajectory changes, forming a hinge-like trace. The Class II condensed history algorithm is used in codes such as in PENetration and Energy LOss of Positrons and Electrons (PENELOPE) [80], GEometry ANd Tracking (GEANT4) [3], and Electron Gamma Shower (EGS) [39].

1.3.4 Production Monte Carlo Electron Transport Codes

This section discusses the background and development of notable production Monte Carlo codes used for electron-photon transport and provides an overview of the methods used in each:

- Electron TRANsport (ETRAN) [83],
- Integrated TIGER Series (ITS) [53],
- Monte Carlo N-Particle (MCNP) [109],
- PENetration and Energy LOss of Positrons and Electrons (PENELOPE) [80],
- GEometry ANd Tracking (GEANT4) [3],
ETRAN is a general-purpose Monte Carlo electron-photon transport that has created a basis for following Monte Carlo electron-photon codes and was developed by Berger and Seltzer in 1963 at the National Bureau of Standards (NBS), which is now the National Institute of Standards and Technology (NIST). The code was originally developed for time-independent electron-transport on simple target geometries of a singular uniform material for energies between to the order of MeV to 1 keV. This energy range was later extended to 1 GeV to 1 keV by including secondary particle production and the coupling with photon and positron transport. The code employs a Class I condensed-history scheme for electron transport and uses the multiple-scatter angular deflection distribution derived by Goudsmit and Saunderson [30] to compute the net angular deflection of a substep length and the energy loss straggling distribution derived by Landau (enhanced by Blunck and Leisegang [7] and Chechin and Ermilova [17]) to compute the net energy loss of a step length.

The framework of ETRAN was later used for the development of the Class I condensed history algorithm in ITS for electron-photon transport at SNL. The development of ITS began in the early 1970's as the TIGER series codes. TIGER involved a series of electron transport codes of differing geometric modeling capabilities for time-independent problems with electron energies ranging from tens of MeV to 1 keV and photon energies ranging from tens of MeV to 10 keV. Similar to the development of ETRAN, this energy range was extended to 1 GeV to 1 keV for both photons and electrons via the inclusion of secondary particle production. Because the maintainence of this series of codes became laborious, ITS was developed to integrate the geometric capabilities of the TIGER series codes into one codebase. Similar to ETRAN, ITS uses the multiple-scattering distributions of Goudsmit and Saunderson and Landau to compute angular deflection and energy loss over a prescribed substep and step length. ITS also has single-scatter electron capabilities.

MCNP is a general-purpose Monte Carlo code developed at Los Alamos National Laboratory (LANL) in 1977. It was initially developed to solve general time-dependent neutral
particle transport problems for arbitrary geometries. MCNP was later upgraded with significant electron transport capabilities in 1997 that can be coupled with neutron and photon transports. This electron transport upgrade employs both single-scatter electron transport and a Class I condensed history algorithm based on the Class I condensed history implementation in ITS. Similar to ETRAN and ITS, the condensed history scheme implemented in MCNP samples from the multiple-scattering distributions of Goudsmit and Saunderson and Landau to compute net angular deflection and energy loss, respectively, for an electron substep and step. At the end of each substep, the production of secondary particles from hard collisions, bremsstrahlung emission, and x-ray are sampled in an analog manner.

PENELOPE is a photon-electron Monte Carlo code developed by Salvat et al. at the University of Barcelona. This code was originally released in 1996 for electron-positron transport with energies of a hundreds of eV to 1 GeV of single-material geometries with quadric surfaces and utilizes the random-hinge method, which falls under the Class II scheme of condensed history methods. Photon transport capabilities were later added. The multi-scattering in this code is handled using the model of Fernandez [28].

GEANT4 was released in 1998 and is an applications-based Monte Carlo code for time-dependent particle transport including electrons, positrons, photons, muons, and hadrons [3]. It was developed for ionizing radiation analysis in applications such as high energy physics, radiotherapy physics, electromagnetic physics, and space-shielding problems. For electron transport, it utilizes a Class II condensed history scheme for an electron energy range as low as 250 eV extending into the TeV energy range. Similar to PENELOPE, the angular deflection of the electron is handled based on the multiple scattering model of Fernandez [28].

EGS is another applications-based Monte Carlo code that was developed in the 1970s at Stanford Linear Accelerator Center (SLAC), specifically, to solve the electromagnetic shower problem [39]. This code was developed using a Class II condensed history algorithm for general geometries of a single homogeneous background material and electron energies between 1 keV and 10 GeV. Electron angular deflection is handled using the multi-scatter
distribution of Goudsmit and Saunderson. EGS was later rewritten as EGSnrc in 2000 with improvements in accuracy of low energy electron cross sections.

1.4  Transport Methods in Stochastic Media

In this section, a review of transport methods developed for transport in stochastic (randomly mixed) media is provided. An important point before proceeding with this discussion is that the researchers of this work were interested in neutral particle transport and not electrons. These methods are reviewed here because they provide a basis for comparing the current methods for binary stochastic media with the analogous method for electron transport that is developed in this dissertation.

In many transport problems, it is sufficient to treat the background as known and homogeneous within a region. In some applications, the background material forms random clumps that must be modeled in some stochastic manner in order to preserve the mean value of the solution. A brute force approach to solving this type of problem would be to perform particle transport on each of many fully generated realizations to compute benchmark solutions, which was an approach proposed by Levermore et al. in 1986 [54]. Though this “benchmark approach” yields exact results in the limit of simulating transport on an infinite number of realizations (with an infinite number of particle histories if using a Monte Carlo approach), it is computationally expensive and not always practical, especially for more complex geometries of higher dimensions and arbitrary mixing containing multiple material types. This large computational expense motivated the development of several approximate but efficient methods that treat the underlying random media in a statistical manner.

1.4.1  Transport Methods in 1D, Binary, Markovian-Mixed Media

Much early attention in this research topic has been in developing a particle transport method for one-dimensional, binary, Markovian-mixed media in which chord lengths of two material types are exponentially distributed [73]. The Atomic Mix (AM) approxi-
mation [22, 73] is the simplest method because it performs transport on a domain where the material properties are homogenized at an atomic level to preserve mean atomic concentrations. This method performs best in applications of finely-mixed, optically thin regions of highly scattering materials. However, the AM approximation generally lacks accuracy for problems in which the material chunk sizes are larger because the effects of the random material-boundary crossings on particle interactions are not adequately captured in a homogenization.

The Levermore-Pomraning (LP) closure [54] is a deterministic method that was developed by Levermore et al. in 1986 to compute the ensemble averaged distribution of particle transport through a purely-absorbing, one-dimensional, binary, Markovian-mixed problem and was demonstrated to yield exact results under those assumptions. This method has an equivalent Monte Carlo method introduced by Adams et al. in 1989 called Chord Length Sampling (CLS) [2, 12, 112], also called Algorithm A (Alg. A) by Zimmerman [112]. CLS samples chord lengths and material types during a particle history but retains no memory of the sampled chord or material after the particle leaves the segment. This method was demonstrated to generally produce more accurate results than the AM approximation for one-dimensional, binary, Markovian-mixed problems with improvement in accuracy for problems with minimal scattering [2, 12]. In the limit of no scattering, CLS produces consistent results with that of the benchmark approach and LP closure.

Variations of Alg. A with improved memory were developed by Zimmerman in 1991 called Algorithm B (Alg. B) and Algorithm C (Alg. C) [112]. Alg. B retains memory of the most recent chord length and material type sampled in the particle history, and Alg. C retains memory of the two most recent chord lengths and material types sampled in the particle history. These memory-enhanced versions each generally produce results of higher accuracy compared to the algorithm from which they were derived.

Conditional Point Sampling (CoPS) [103] is a Monte Carlo algorithm developed by Vu and Olson in 2019 that uses delta (or Woodcock) tracking [108] to stream particles in a do-
main without defined geometric features. Delta tracking tracks particles using the majorant cross section to sample distances to candidate collisions. Then, a collision is sampled based on the ratio of the actual cross section to the majorant, which enables particles to cross multiple material regions without fully generating material realizations. The CoPS algorithm samples and preserves memory of the material type of discrete points conditionally on neighboring points on-the-fly. Unlike the other approximate methods mentioned, CoPS is able to easily compute the variance of the mean caused by the randomness of material mixing and is not specific to one type of material mixing. The accuracy of the algorithm relies solely on the fidelity of a derived conditional probability function. For Markovian-mixed media, this conditional probability function was derived based on a “pseudo-interface” concept of generating material realizations [71], where cell boundaries in a realization are defined by randomly placing pseudo-interfaces and their material types are randomly sampled based on the abundance of each material. Though the method has been demonstrated to produce highly-accurate mean results for one-dimensional, binary, Markovian-mixed media [103], the algorithm relies on a growing list of material types and locations that are sorted through during simulation, which can cause unbounded increases in computer memory requirement and runtime. Limited-memory versions of CoPS including analogous algorithms to CLS, Alg. B, and Alg. C have been studied for runtime and accuracy trade-offs using one-dimensional, binary, Markov problems in 2020 and 2021 [101, 102].

1.4.2 Transport Methods in Multi-Dimensional, Binary, Stochastic Media

Recent work has been in expanding existing transport methods for 1D, binary, Markovian-mixed media to 3D, binary, Markovian-mixed media. Because the AM approximation homogenizes material properties, it easily extends to higher-dimensional problems as well as problems with different material-mixing statistics. AM approximation benchmarks for multi-dimensional, binary, Markov mixtures were produced by Larmier et al. in 2017 [48]. CLS and Alg. B were also extended to multi-dimensional, binary, Markovian-mixed media by
Larmier et al. [48] and Brantley et al. [14], respectively, in 2017. The multi-dimensional implementation of Alg. B was called Local Realization Preserving (LRP) [14]. Though Alg. C has improved accuracy compared to Alg. B, the method is more difficult to extend to multi-dimensional problems. CoPS was also extended to multi-dimensional, binary, Markovian-mixed media by Olson and Vu in 2019 [69].

Additional work has been done in expanding computing capabilities for problems of other mixing statistics and higher dimensions. Brantley and Martos produced benchmarks for binary, three-dimensional stochastic media problems containing spherical inclusions of varying mean chord lengths and sphere radii distributions with an optically thin background material in 2011 [13]. In addition to Markovian mixtures, Larmier et al. produced benchmark solutions for Voronoi-mixed, and Cartesian-box-mixed problems of three-dimensional, binary material composition using Poisson-Voronoi tessellations and Poisson-Box tessellations, respectively, in 2017 [49]. Isotropic Poisson tessellations utilize randomly oriented, Poisson-distributed hyperplanes to define potential material boundaries. Poisson-Voronoi tessellations rely on randomly placed points called “seeds” within the domain to define each Voronoi cell, which is the set of points closest to that seed compared to any other seed. Poisson-Box tessellations decompose the domain into a set of Cartesian boxes defined by Poisson-distributed hyperplanes sampled and oriented in Cartesian-coordinate directions. In the work of Larmier et al., the authors provided an accuracy comparison of transport results in binary, Markovian-mixed problems against transport results in Voronoi-mixed and Cartesian-box-mixed problems and found that, for the problems investigated in their work, binary, Markovian-mixed media was an accurate model for Cartesian-box-mixed geometries and produced nearly identical results but resulted in significant differences when compared against Voronoi-mixed problems.

Poisson-Box Sampling (PBS) [50] is a Monte Carlo method developed by Larmier et al. in 2018 for binary, multi-dimensional, box-mixed problems. The algorithm samples the material type of Cartesian boxes on-the-fly. PBS-1 and PBS-2 are variants of the PBS algorithm that
are analogous to CLS and LRP in that PBS-1 commits the material type of the most recently sampled Cartesian box to computer memory and PBS-2 commits the two most recent.

1.4.3 Transport Methods in N-ary Stochastic Media

In addition to expanding transport in stochastic media capabilities to multiple dimensions and other material mixing statistics, work has also be done in handling stochastic mixing between more than two materials. The LP closure was generalized by Pautz and Franke for one-dimensional, N-ary, Markov geometries in 2015 [70]. Later in 2021, a theory was developed by Olson et al. [68], which was used to extend CLS and LRP to Markovian-mixed media of N-ary mixing in one-dimension by Vu et al. [98].

1.5 Electron Transport Methods for Stochastic Media

Many methods have been developed for modeling neutron transport in stochastic media and can be directly applied to photons in stochastic media. While these approaches could be applied directly to single-scatter electron transport, they are not directly applicable to condensed history models. Limited work has been done in modeling electron-photon transport in stochastic media and are reviewed here.

Levermore and Zimmerman derived an expression for the fraction of charged fusion reaction products in a fuel mixture in the fuel region of an ICF target using a binary Markovian model [55]. This work applies to heavy charged particles but does not directly apply to electrons because of their lower mass, which would require considering additional physical effects

Franke et al. investigated the accuracy of the condensed history Monte Carlo electron transport algorithm used in ITS on stochastic media electron transport problems [29]. The authors evaluated the accuracy of the condensed history algorithm in handling material boundary crossings by introducing artificial material boundaries in a pure material to induce the material boundary crossing mechanism in each algorithm. The accuracy of this algorithm
was also investigated in modeling electron transport on stochastic geometries with several material boundary crossings by benchmarking energy deposition and leakage results against single-scatter simulations. The algorithm relied on multiple-scattering distributions that assumed a uniform background material to step through material boundary crossings, and the learnings from this work resulted in improvements on the algorithm to make more accurate approximations in the electron energy loss and angular deflection at a material crossing as a result of substep truncation. What differs between the work of Franke et al. and the work introduced in this dissertation is that this work aims to develop a condensed history method that can accurately handle the random material boundary crossings that may occur within an electron substep without the need for truncation within a stochastic mixture.

Larsen and Liang [51] showed that the AM approximation is accurate for problems in which the transport mean free path is significantly larger than the material mean chord lengths. The authors conducted a theoretical asymptotic analysis on charged particle transport problems devoid of hard collisions such that the charged particle would only experience small changes in direction and energy. The authors showed that this type of problem is a formal asymptotic limit of the linear Boltzmann equation and derived an expression identical to the equation as a result of applying the AM approximation to the linear Boltzmann equation, extending the range of applicability of the AM approximation to charged particle transport problems in stochastic media. However, this work does not account for charged particle transport problems in which hard collisions have a significant effect on transport results in a stochastic mixture. This work also does not extend the range of validity of the AM approximation to problems where the material mean chord length and transport mean free path are of comparable lengths.

In summary, while the field of stochastic transport for neutral particles and the field of numerical methods for electron transport are quite mature independent of each other, there have yet to be any serious attempts to develop methods for electron transport specifically. This dissertation will fill this gap by constructing a condensed history method applied to
1.6 Outline of Dissertation

Chapter 2 describes the physics of individual photon and electron interactions that would be modeled in a single-scatter Monte Carlo simulation. Governing equations and common approximations are introduced, and solution techniques (not including the Condensed History method) are described.

Chapter 3 reviews the theories and methods used in a Class I condensed history algorithm for a homogeneous background material. This chapter derives the multi-scatter distributions used to sample the energy loss over an electron step, multi-scatter distributions used to sample the angular deflection over an electron substep, and describes how the production of secondary particles are handled in a Class I condensed history algorithm.

Chapter 4 derives multi-scatter distributions described in Chapter 3 that are applicable to stochastic media, establishing the primary original scientific contribution of this dissertation. The multi-scatter distribution derivations for energy loss and angular deflection are generalized to account for a stochastic mixture in which more than one material type may be traversed within an electron substep, and methods for handling secondary particle production in stochastic media are introduced.

Chapter 5 introduces the condensed history code developed in this dissertation called the Stochastic Mixture Accounted Condensed History Electron (SMACHE) method (pronounced “smash”). This chapter presents numerical results on a set of benchmark problems, quantifying the accuracy of the methods developed in Chapter 4 relative to benchmark calculations using single scatter and condensed history models with explicit random material boundaries.

Chapter 6 summarizes the findings of this dissertation and provides a discussion of future research avenues.
CHAPTER 2

Photon-Electron Transport Theory

When developing an electron transport method, it is necessary to account for both photon and electron transport because these particles can produce secondary photons and electrons as they interact with matter. This chapter begins by detailing the physical processes of electron and photon interactions and provides the corresponding differential cross section (DCS). Unlike neutron DCS, which are acquired from experimental measurements, the DCS of electron and photon interactions can be derived based on quantum mechanical principles. This chapter then establishes the governing coupled photon-electron transport equation valid for single scattering and the Boltzmann Fokker-Planck (BFP) using these interactions. Solution techniques to solve these equations are also described.

For the remainder of this document, we define the following terms and constants:

\[ \beta = \frac{\sqrt{E(E + 2m_e c^2)}}{E + m_e c^2}, \]  
(2.1)

\[ \kappa = \frac{E}{m_e c^2}, \]  
(2.2)

\[ \gamma = \frac{E + m_e c^2}{m_e c^2}, \]  
(2.3)

\[ \mu = \cos \theta, \]  
(2.4)

\[ r_e = \frac{e^2}{m_e c^2}, \]  
(2.5)

\[ \alpha = \frac{e^2}{4\pi \epsilon_0 \hbar c}. \]  
(2.6)
where $E$ is the kinetic energy of the incident particle, $m_e c^2 = 0.511$ MeV is the rest mass energy of the electron, $c$ is the speed of light, $\theta$ is the outgoing angle of the scattered particle relative to the incident particle direction and $\mu \in [-1, 1]$, $r_e$ is the classical electron radius, $e$ is the elementary charge of an electron, $\alpha$ is the fine structure constant, which describes the strength of electron electromagnetic interactions, $\epsilon_0$ is the permittivity of free space, and $\hbar$ is the reduced Planck constant.

We also establish select basis functions that form a set of orthogonal functions that can be used to exactly express functions that are used throughout this chapter and this work when no truncations are introduced. We begin with the recursion relation of Legendre polynomials $P_n(\mu)$, which are used in defining the associated Legendre polynomials $P^m_n(\mu)$ and spherical harmonic functions. We also discuss Bessel functions and modified Bessel functions, which are written in spherical coordinates. The recursion relation of Legendre polynomials is

$$
\mu P_n(\mu) = \frac{(n + 1)P_{n+1}(\mu) + nP_{n-1}(\mu)}{2n + 1}, \quad 0 \leq n < \infty, \quad (2.7a)
$$

where $\hat{\Omega} = \langle \mu, \phi \rangle$ is the directional unit vector and $\phi$ is the azimuthal angle. The first three Legendre polynomials are

$$
P_0(\mu) = 1, \quad (2.7b)
$$

$$
P_1(\mu) = \mu, \quad (2.7c)
$$

$$
P_2(\mu) = \frac{1}{2}(3\mu^2 - 1). \quad (2.7d)
$$

The orthogonality condition for Legendre polynomials is

$$
\int_{-1}^{1} P_n(\mu)P_m(\mu)d\mu = \frac{2}{2n + 1}\delta_{n,m}. \quad (2.7e)
$$
Using the Legendre polynomials, any function $f(\mu)$ can be expanded in an infinite sum:

$$f(\mu) = \sum_{n=0}^{\infty} \frac{2n+1}{2} f_n P_n(\mu), \quad -1 \leq \mu \leq 1,$$

(2.7f)

$$f_n = \int_{-1}^{1} P_n(\mu') f(\mu') d\mu'.$$

(2.7g)

The associated Legendre polynomials can be expressed in terms of Legendre polynomials:

$$P_n^m(\mu) = (1 - \mu^2)^{m/2} \left( \frac{d}{d\mu} \right)^m P_n(\mu), \quad 0 \leq m \leq n < \infty,$$

(2.8)

and are used in the expressions of the spherical harmonics functions, which are defined on a spherical surface:

$$Y_n^m(\hat{\Omega}) = \left[ \frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!} \right]^{1/2} \frac{P_n^{|m|}(\mu) e^{im\phi}}{(n!)^{|m|}} Y_m(\hat{\Omega}), \quad 0 \leq |m| \leq n < \infty,$$

(2.9a)

$$e^{im\phi} = \cos(m\phi) + i \sin(m\phi).$$

(2.9b)

The spherical harmonics functions can be used to expand any function $f(\hat{\Omega})$ defined on a unit sphere:

$$f(\hat{\Omega}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} f_{n,m} Y_n^m(\hat{\Omega}),$$

(2.9c)

$$f_{n,m} = \int_{4\pi} f(\hat{\Omega}) Y_n^{-m}(\hat{\Omega}) d\Omega,$$

(2.9d)

and satisfy the orthogonality condition

$$\int_{4\pi} Y_n^m(\hat{\Omega}) Y_k^{-l}(\hat{\Omega}) d\Omega = \delta_{n,k} \delta_{m,l}.$$

(2.9e)
The Legendre polynomials are recovered using the Legendre addition theorem, also called the spherical harmonic addition theorem:

\[
P_n(\hat{\Omega} \cdot \hat{\Omega}') = \frac{4\pi}{2n+1} \sum_{m=-n}^{n} Y_n^m(\Omega)Y_n^{-m}(\Omega') = P_n(\mu_1)P_n(\mu_2) + 2\sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} P_m^m(\mu_1)P_m^m(\mu_2) \cos[m(\phi_1 - \phi_2)]. \tag{2.10}
\]

Bessel functions, which are written in cylindrical coordinates, are solutions to Bessel’s differential equation

\[
x^2 \frac{d^2y}{dx^2} + x \frac{dy}{dx} + (x^2 - n^2) y = 0, \tag{2.11a}
\]

where \( n \) is the order of the Bessel function. Bessel functions of the first kind take the form

\[
J_n(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!(m+n)!} \left( \frac{x}{2} \right)^{2m+n}. \tag{2.11b}
\]

The modified Bessel functions of the first kind are expressed in terms of Bessel functions of the first kind:

\[
I_n(x) = i^{-n}J_n(ix). \tag{2.11c}
\]

### 2.1 Electron Interactions

The transport of electrons and photons are fundamentally different from each other on the count of the former being charged and the latter being neutral, bringing about the significant difference in mean free path. Unlike photons, which traverse materials with simple free flight between relatively intermittent interactions, electrons lose energy as they travel through matter and can have a substantial number of collisions within a short length-scale due to the long-range Coulomb force that dominates its flight. The electron interactions of
interest are elastic scattering, inelastic scattering, Bremsstrahlung emission, and positron annihilation.

### 2.1.1 Elastic Collisions

During an electron elastic collision, illustrated in Figure 2.1, an incident electron with kinetic energy $E$ is deflected by a nearby nucleus with negligible energy loss and a change in direction. Unlike hard sphere scattering where the incident particle collides directly with

![Figure 2.1: Electron elastic scattering process [80]](image)

the target nuclei, the elastic scattering of electrons is driven by the repulsive Coulomb force between the incident electron and the orbital electrons of the background nuclei. These collisions occur frequently as an electron transports through a background material, especially at high kinetic energies and in high $Z$ materials. Because the Coulomb forces felt by the electron from the background material must be considered, the incident electron trajectory cannot be computed assuming hard collision mechanics. The Rutherford scattering DCS [78] accounts for this Coulomb force and is

$$
\frac{d\sigma}{d\Omega_{Ruth}} = \frac{z_1^2 z_2^2 \alpha^2 (hc)^2}{16 E^2 \sin^4(\theta/2)},
$$

(2.12)

where $z_1$ and $z_2$ are the charge number of the projectile particle and the target nuclei. For an electron, $z_1 = -1$.

The Rutherford scattering DCS does not account for quantum effects, which are pertinent
for electrons with kinetic energies $E > 1$ keV. For energies greater than 1 keV, quantum mechanical processes must be included in the electron elastic scattering DCS. Mott derived a DCS that considers spin and relativistic effects [64]:

$$\frac{d\sigma}{d\Omega_{\text{Mott}}} = |f(\theta)|^2 + |g(\theta)|^2,$$

(2.13a)

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} P_l(\cos \theta) \left\{ (l + 1)[\exp(2i\delta_{l+}) - 1] + l[\exp(2i\delta_{l-}) - 1] \right\},$$

(2.13b)

$$g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} P^1_l(\cos \theta) \left\{ \exp(2i\delta_{l-}) - \exp(2i\delta_{l+}) \right\},$$

(2.13c)

$$k = \frac{1}{\hbar c} \sqrt{E(E + 2m_e c^2)},$$

(2.13d)

where $P_l(\cos \theta)$ are Legendre polynomials, $P^1_l(\cos \theta)$ are associated Legendre functions, $\delta_{l\pm}$ are phase shifts [79, 105], $f(\theta)$ is the direct scattering amplitude, $g(\theta)$ is the spin-flip scattering amplitude, and $k$ is the projectile wave number. This elastic scattering DCS can be computed using the Partial-Wave method for energies ranging from 1 keV to 300 keV, which can be computationally demanding because of the hundreds of phase shifts that may be considered in the calculation. Production electron transport codes typically rely on tabulated elastic scattering DCSs of Riley et al. [76] for energies from 1 keV to 256 keV.

For electron kinetic energies greater than 300 keV, screening effects from orbital electrons must also be considered in addition to spin and relativistic effects. Seltzer [84] formulated a DCS as a function of the Mott DCS and Rutherford DCS, which accounts for screening effects [78]:

$$\frac{d\sigma}{d\Omega} = \frac{Z^2 e^2}{p^2 v^2 (1 - \mu + 2\eta)^2} \left[ \frac{(d\sigma/d\Omega)_{\text{Mott}}}{(d\sigma/d\Omega)_{\text{Ruth}}} \right],$$

(2.14a)

$$\eta = \frac{1}{4} \left( \frac{\alpha m_e c}{0.885 p} \right)^2 Z^{2/3} \left[ 1.13 + 3.76 \left( \frac{\alpha Z}{\beta} \right)^2 \sqrt{\frac{\kappa}{\kappa + 1}} \right],$$

(2.14b)

where $p$ is the momentum of the electron, $v$ is the velocity of the electron, and $\eta$ is a modification of Moliere’s [61] formulated screening correction proposed by Seltzer [84].
note that the ratio \((d\sigma/d\Omega)_{\text{Mott}}/(d\sigma/d\Omega)_{\text{Rath}}\) was reformulated by Boschini et al. [11] for improved numerical evaluation and tabulated for select elements and energies:

\[
\frac{(d\sigma/d\Omega)_{\text{Mott}}}{(d\sigma/d\Omega)_{\text{Rath}}} = \frac{2(1-\mu)}{(\kappa+1)^2} \left| F \right|^2 + \frac{|G|^2}{(\alpha' z Z)^2} \frac{2p^2(1-\mu)^2}{(\kappa+1)^2(1+\mu)},
\]  

(2.15a)

\[
F = F_0 + F_1,
\]  

(2.15b)

\[
G = G_0 + G_1,
\]  

(2.15c)

where

\[
F_0 = -\frac{R}{iq},
\]  

(2.16a)

\[
G_0 = R \cot^2 \left( \frac{\theta}{2} \right),
\]  

(2.16b)

\[
F_1 = \frac{i}{2} \sum_{l=0}^{\infty} \left[ l D_l + (l+1) D_{l+1} \right] (-1)^l P_l(\mu),
\]  

(2.16c)

\[
G_1 = \frac{i}{2} \sum_{l=0}^{\infty} \left[ l^2 D_l - (l+1)^2 D_{l+1} \right] (-1)^l P_l(\mu),
\]  

(2.16d)

and

\[
R = \frac{q}{2} \frac{\Gamma(1-iq)}{\Gamma(1+iq)} \exp \left[ 2iq \ln \left( \sin \frac{\theta}{2} \right) \right],
\]  

(2.17a)

\[
D_l = \frac{\exp(-i\pi \xi_l) \Gamma(\xi_l - iq)}{\xi_l + iq} \frac{\exp(-i\pi l) \Gamma(l - iq)}{l + iq} \frac{\Gamma(l + iq)}{\Gamma(l + iq)},
\]  

(2.17b)

\[
\xi_l = \sqrt{l^2 - (\alpha')^2},
\]  

(2.17c)

\[
q = \frac{\alpha'}{\beta},
\]  

(2.17d)

\[
\alpha' = -\alpha z Z,
\]  

(2.17e)

and \(z\) is the charge number of the incident particle.

In this work, the tabulated DCS of Riley et al. [76] are used for electron energies 1 keV to 256 keV. For energies greater than 256 keV, DCSs were computed using Eqs. (2.14) and
2.1.2 Inelastic Collisions

Occasionally, an electron can interact directly with another electron and experience an inelastic collision, often called a hard collision. The electron inelastic collision is a process by which an incident electron with kinetic energy $E$ excites and ionizes an orbital electron, typically assumed to be a free electron, such that the $i^{th}$ shell binding energy $U_i$ is negligible. During this collision, the primary electron transfers some of its kinetic energy $W$ to the secondary electron and experiences a change in direction. This interaction becomes more abundant at lower kinetic energies and is shown in Figure 2.2.

![Figure 2.2: Electron inelastic scattering process](image)

The DCS for a hard collision by an electron was derived by Møller [62] by taking the sum of collisions with each orbital electron of the nucleus:

$$
\frac{d\sigma_{in,e}}{d\epsilon} = \frac{2\pi e^4}{m_e c^2 \beta^2 E} \frac{1}{\epsilon^2 + \frac{1}{(1-\epsilon)^2}} + \left( \frac{\kappa}{\kappa + 1} \right)^2 - \frac{2\kappa + 1}{(\kappa + 1)^2} \frac{1}{\epsilon(1-\epsilon)},
$$

(2.18)

where $\epsilon = W/E$ is the fraction of the electron kinetic energy transferred. This derivation assumes that the target electron receives all of the momentum transfer rather than sharing the momentum transfer with the nucleus. Normalizing this DCS by the total inelastic scattering cross section yields the probability density function of the energy transfer to the secondary electron.
electron:

\[
g_e(\epsilon, \epsilon_c)d\epsilon = \frac{1}{\sigma_{in,e}(\epsilon_c)} \frac{d\sigma_{in,e}}{d\epsilon}d\epsilon, \tag{2.19a}
\]

\[
\sigma_{in,e}(\epsilon_c) = \frac{2\pi e^4}{m_e c^2 \beta^2} E \left[ \frac{1}{\epsilon_c} - \frac{1}{1 - \epsilon_c} + \left( \frac{\kappa}{\kappa + 1} \right)^2 \left( \frac{1}{2} - \epsilon_c \right) - \frac{2\kappa + 1}{(\kappa + 1)^2} \ln \left( \frac{1 - \epsilon_c}{\epsilon_c} \right) \right], \tag{2.19b}
\]

where \(\epsilon_c\) is the energy cutoff fraction of the secondary electron (typically 1 keV).

For energies \(E > 1\) keV, positrons may also experience an inelastic collision that results in the production of a secondary electron. This interaction differs from a hard collision of an electron because of the positive charge of the positron and must account for significant exchange effects. The DCS for a hard collision by a positron was derived by Bhabha [6]:

\[
\frac{d\sigma_{in,p}}{d\epsilon} = \frac{\epsilon_c}{(\kappa - 1)^2(\kappa + 1)\epsilon^2} \left[ 1 + 2(\kappa - 1)(1 - \epsilon) + (\kappa - 1)^2 \left( 1 - \epsilon + \frac{1}{2} \epsilon^2 \right) \right], \tag{2.20}
\]

and similarly to hard collisions by electrons, the probability density function of the energy transfer is computed by normalizing the DCS by the total inelastic scattering cross section:

\[
g(\epsilon, \epsilon_p)d\epsilon = \frac{1}{\sigma_{in,p}(\epsilon_c)} \frac{d\sigma_{in,p}}{d\epsilon}d\epsilon, \tag{2.21}
\]

\[
\sigma_{in,p}(\epsilon_c) = \frac{\epsilon_c}{(\kappa - 1)^2(\kappa + 1)} \left[ \frac{\kappa^2 \epsilon_c^2}{2} + 2 \epsilon_c - 3 + \ln(\epsilon_c)(\kappa^2 - 1) + \left( \kappa - \frac{1}{2} \right)(1 - \epsilon_c) \right]. \tag{2.22}
\]

Once the outgoing energy \(W\) of the secondary particle is determined, momentum conservation is used to determine the outgoing polar scattering angle:

\[
\mu = \left[ \left( \frac{E - W}{E} \right) \left( \frac{E + 2m_e c^2}{E - W + 2m_e c^2} \right) \right]^{1/2}. \tag{2.23}
\]
2.1.3 Bremsstrahlung Emission

Bremsstrahlung (or braking radiation) emission is a process by which an incoming electron of kinetic energy $E$ is decelerated by the electric field of a target nuclei because of the attractive force between the primary electron and positive charge of the target nucleus and the repulsive force between the primary electron and the negative charge of the background electrons. During this deceleration, the primary electron is deflected, and the energy loss $W$ is conserved in the form of a photon. The energy loss can range between 0 and $E$ and loses more energy the closer it passes through the target nucleus. This process typically occurs when high energy electrons transport through high $Z$ materials, and is depicted in Figure 2.3.

![Bremsstrahlung emission](image)

Figure 2.3: Bremsstrahlung emission process [80]

The bremsstrahlung DCS accounts for the contribution of electron deceleration from the nucleus $d\sigma_n/dW$ and field electrons $d\sigma_e/dW$. Many approximations of the bremsstrahlung DCS have been developed for various energy regimes. One approximation is the sum

$$\frac{d\sigma_{br}}{dW} \approx \frac{d\sigma_n}{dW} + Z\frac{d\sigma_e}{dW}, \quad (2.24)$$

$$\frac{d\sigma_n}{dW} = \frac{4\alpha r_e^2 Z^2}{W}(\chi_{Born}^{unscr} + \delta_{screen} + \delta_{Coul}), \quad (2.25)$$

$$\frac{d\sigma_e}{dW} = \frac{4\alpha r_e^2}{W}(f_e - \chi_{Haug} + \delta_{screen}^e), \quad (2.26)$$
where $\chi_{\text{Born}}^{\text{unscre}}$ is the well-known Bethe-Heitler Born-approximation solution of an unscreened nucleus [45], $\delta_{\text{screen}}$ is the screening correction factor of the nucleus, $\delta_{\text{Coul}}$ is the Coulomb correction factor of the nucleus, $f_{e-e}$ is the Coulomb correction correction factor of the field electrons [60], $\chi_{\text{Haug}}$ is the Haug Born-approximation solution of an unscreened free electron [32], and $\delta_{e\text{screen}}$ is the screening correction factor of the field electrons.

The Bethe-Heitler Born approximation formulation accounts for screening and assumes that the kinetic energy of the electron is much larger than the rest mass energy of an electron $m_e c^2$ before and after the bremsstrahlung emission process, which is valid for most physical processes [80]:

$$\frac{d\sigma_{\text{born}}^\text{br}}{dW} = r_e^2 \alpha Z (Z + \eta) \frac{1}{W} \left[ \epsilon^2 \varphi_1(b) + \frac{4}{3} (1 - \epsilon) \varphi_2(b) \right], \quad (2.27a)$$

$$\varphi_1(b) = 4 \ln \left( \frac{R m_e c}{\hbar} \right) + 2 - 2 \ln(1 + b^2) - 4 b \arctan(b^{-1}), \quad (2.27b)$$

$$\varphi_2(b) = 4 \ln \left( \frac{R m_e c}{\hbar} \right) + \frac{7}{3} - 2 \ln(1 + b^2) - 6 b \arctan(b^{-1})$$

$$- b^2 [4 - 4 b \arctan(b^{-1}) - 3 \ln(1 + b^{-2})], \quad (2.27c)$$

$$b = \frac{R m_e c}{\hbar} \frac{\epsilon}{2 \gamma \left( 1 - \epsilon \right)}, \quad (2.27d)$$

$$\epsilon = \frac{W}{E + m_e c^2}, \quad (2.27e)$$

where $\hbar = h/2\pi$ is the reduced Planck’s constant, $R$ is the screening radius, and $\eta$ is the bremsstrahlung production factor in the atomic electrons field [82]. Koch and Motz [45] published a more extensive collection of bremsstrahlung DCS theoretical formulations derived under various assumptions for low-energy and high-energy regimes, which were then consolidated by Seltzer and Berger to produce a comprehensive set of scaled Bremsstrahlung DCS $\chi_{\text{scaled}}$ [86, 87] widely used in production electron transport codes:

$$\frac{d\sigma_{\text{br}}}{dW} = \frac{Z^2}{\beta^2 W} \chi_{\text{scaled}}. \quad (2.28)$$
Once the outgoing kinetic energy of the photon is sampled, the angular deflection can be sampled. The probability density function of $\mu = \cos \theta$ has be formulated under various assumptions and takes many forms [1, 37, 41, 42, 88].

2.1.4 Positron Annihilation

A positron is produced from the photon interaction pair production, described in Section 2.2.4. Positron annihilation, depicted in Figure 2.4, is the process by which a low energy positron with energy $E$ collides with a free electron and emits two photons of energy $E_-$ and $E_+$ in directions $\mu_- = \cos(\theta_-)$ and $\mu_+ = \cos(\theta_+)$. This process conserves energy and momentum such that $E_- + E_+ = E + 2m_e c^2$. The positron annihilation DCS was derived by Heitler [33] in the center-of-mass frame [80]. This derivation was later used by Nelson et al. [67] to derive the positron annihilation DCS in the laboratory frame such that the target electron is at rest:

$$\frac{d\sigma_{an}}{d\zeta} = \frac{\pi r_e^2}{(\gamma + 1)(\gamma^2 - 1)} [S(\zeta) + S(1 - \zeta)], \quad (2.29a)$$

$$S(\zeta) = -(\gamma + 1)^2 + (\gamma^2 + 4\gamma + 1)\frac{1}{\zeta} - \frac{1}{\zeta^2}, \quad (2.29b)$$

$$\zeta = \frac{E_-}{E + 2m_e c^2}, \quad (2.29c)$$
where $\gamma$ is the total energy of the positron in rest energy units. Using this DCS, the energies of the outgoing photons can be determined such that conservation of energy, $E_- + E_+ = E + 2m_e c^2$, is satisfied. Momentum is conserved by the relationship

$$\mu_- = \frac{\gamma + 1 + \zeta^{-1}}{\sqrt{\gamma^2 - 1}},$$  \hspace{1cm} (2.30a)

$$\mu_+ = \frac{\gamma + 1 + (1 - \zeta)^{-1}}{\sqrt{\gamma^2 - 1}},$$  \hspace{1cm} (2.30b)

$$\phi_+ = \phi_- + \pi,$$  \hspace{1cm} (2.30c)

where the polar angle $\phi_-$ is azimuthally symmetric.

In this work, it is assumed that the incoming positron has negligible momentum at the time of collision because positron annihilation occurs at low energies such that the particle is essentially at rest. Under this assumption, only the rest mass energy of the positron and target electron are conserved in the resulting photon pair, each produced with energy $E_+ = E_- = m_e c^2$. By conservation of momentum, the outgoing directions of the produced photons must be exactly opposite of each other and are isotropically sampled.

### 2.1.5 Electron Stopping Power

Electrons can lose energy to ionization and excitations as a result of inelastic collisions (collisional energy loss) and to the production of electromagnetic radiation (radiative energy loss) as it moves through matter. The mean collisional and radiative energy loss rates of an electron can be described with their respective stopping power, which is defined as [84]:

$$-\left( \frac{dE}{dx} \right)_{col} = N \int_0^E W \frac{d\sigma_{in}}{dW} dW,$$  \hspace{1cm} (2.31)

$$-\left( \frac{dE}{dx} \right)_{rad} = N \int_0^E W \frac{d\sigma_{re}}{dW} dW.$$

32
where $N$ is the target number density, $W$ is the energy loss of the primary electron, $\sigma_{in}$ is the cross section of the inelastic scattering cross section for collisional energy losses, and $\sigma_{br}$ is the bremsstrahlung emission cross section for radiative energy losses. These stopping powers evaluate to be [5]

$$\left(\frac{dE}{dx}\right)_{col} = \frac{2\pi e^4 NZ}{m_e c^2 \beta^2} \left\{ \ln \left[ \frac{\tau^2 (\tau + 2)}{4 I^2} \right] - \beta^2 + 1 + \left[ \frac{1}{8} + \ln(2) \right] \left( \frac{\tau}{\tau + 1} \right)^2 - \delta \right\}, \quad (2.33)$$

$$\left(\frac{dE}{dx}\right)_{rad} = N \alpha r^2 Z^2 (E + m_e c^2) \Phi_{br}, \quad (2.34)$$

where $I$ is the mean ionization energy, $\delta$ is the density effect correction factor (further discussed in Section 2.1.6), and $\Phi_{br}$ is the scaled bremsstrahlung cross section. The total energy loss rate of the electron is characterized by the total mean stopping power, which is the sum of the collisional and radiative stopping powers:

$$\left(\frac{dE}{dx}\right)_{tot} = \left(\frac{dE}{dx}\right)_{col} + \left(\frac{dE}{dx}\right)_{rad}. \quad (2.35)$$

### 2.1.6 Density Effect Correction

The density effect correction $\delta$ is used to account for the effects of the electric field of the electron, which polarizes background electrons and distorts the negative electric charge. In this process, the interaction between the primary electron and distant background electrons is screened by nearby polarized background electrons such that the energy loss of the primary electron from collisions is reduced. This reduction in collisional stopping power is reflected in the density effect correction factor, which was derived by Fano [25, 26] as a function of material optical data:

$$\delta = \frac{2}{\pi \omega_p^2} \int_0^\infty \omega d\omega \text{Im} \left[ -\frac{1}{\epsilon(\omega)} \right] \ln \left( 1 + \frac{l^2}{\omega^2} \right) - \left( \frac{l}{\omega_p} \right)^2 (1 - \beta^2), \quad (2.36)$$

33
where \( \omega_p = \sqrt{\frac{4\pi e^2}{m}} \) is the plasma frequency, \( l \) is the root of \( 1 - \beta^2 \epsilon(il) = 0 \), and \( \epsilon(\omega) \) is the dielectric-response function of the medium. Because input data for a considerable amount of materials is not readily available for this formulation of the density effect correction, Sternheimer [89] proposed another expression of the density effect correction

\[
\delta = \sum_{i=1}^{n} f_i \ln \left( 1 + \frac{l^2}{\left( \frac{\mu_{St} E_i}{\hbar \omega_p} \right)^2 + \alpha_i f_i} \right) - l^2 (1 - \beta^2),
\]

(2.37)

\[
\frac{1}{\beta^2} - 1 = \sum_{i=1}^{n} \frac{f_i}{(h\omega_p)^2 + \alpha_i f_i},
\]

(2.38)

\[
2 \ln \left( \frac{I}{\hbar \omega_p} \right) = \sum_{i=1}^{n} f_i \ln \left( \frac{\mu_{St} E_i}{\hbar \omega_p} + \alpha_i f_i \right),
\]

(2.39)

which requires knowledge of the material binding energies \( E_i \), oscillator strengths \( f_i \), and mean excitation energy \( I \). Here, \( l \) is the root of Eq. (2.38) and \( \mu_{St} \) satisfies Eq. (2.39).

### 2.2 Photon Interactions

A photon is a massless, chargeless particle that can also be described as a packet of electromagnetic waves or light. Unlike charge particles, photons do not interact with the Coulomb forces of background materials and thus do not continuously lose energy as they transport through materials. As a photon moves through matter, it can experience photoelectric absorption, coherent (Rayleigh) scattering, incoherent (Compton) scattering, and electron-positron pair production. Generally, coherent scatters occur less frequently relative to incoherent scatters, photoelectric absorptions, and pair production. The frequency of these interactions are dependent on the photon energy \( E \), and the atomic number \( Z \) of the background material that the photon is transporting through. This relationship is shown in Figure 2.5. In this work, tabulated photon data from the MCNP6 file mcplib84 was used.
2.2.1 Photoelectric Effect

The photoelectric effect, illustrated in Figure 2.6, is a photon interaction dominant in the low-energy regime. It can be described as the ionization of an electron bound to a target nuclei by an incident electromagnetic wave (or light) of a great enough frequency. Through this phenomenon, light was observed by Einstein to obey wave-particle duality and deposit discrete amounts of energy in the form of a photon [23]. The energy of a photon can be expressed as 

$$E = h\nu,$$

where $h$ is Planck’s constant and $\nu$ is the frequency of the electromagnetic wave. For a photon of energy $E$ to eject an electron in the $i^{th}$ shell, its energy must exceed the electron binding energy $U_i$, often referred to as the work function, the minimum energy required to eject the electron. Energy is conserved, and the energy of the ionized electron is $E_e = E - U_i$. If an electron in a lower energy shell is ionized by an incoming photon, an electron residing in a higher energy orbital may relax and fill this vacancy, causing the target nuclei to fluoresce. Fluorescence is neglected in this work. The scattering angle $\theta_e$ of a $k$-shell electron follows an angular distribution that derives from the
photoelectric DCS, expressed by Sauter [80, 81] as

\[
d\sigma_{ph} = \alpha^2 r_e^2 \left( \frac{Z}{\kappa} \right)^2 \frac{1 - \mu^2}{(1 - \beta \mu)^4} \left[ 1 + \frac{1}{2} \gamma(\gamma - 1)(\gamma - 2)(1 - \beta \mu) \right],
\]

\( \gamma = 1 + \frac{E_e}{m_e c^2}. \)

### 2.2.2 Coherent (Rayleigh) Scattering

The Rayleigh scattering process, shown in Figure 2.7 occurs at lower energies \((E < 10 \text{ keV})\) and is infrequent compared to photoelectric absorption. During this interaction, a photon collides with a bound outer shell electron of a heavy nucleus. The energy from the incident photon is absorbed by the nucleus and excites the outer shell electron. There is not enough energy to eject the electron, so no ionization of the atom occurs. Upon relaxation, the electron emits a photon of the same energy in a different outgoing direction.

The Rayleigh scattering DCS derives from Thomson scattering, which is the elastic scattering of a classical electromagnetic wave by a single free electron at low incident energies. The DCS of Thomson scattering is

\[
d\sigma_T = \frac{r_e^2}{2} (1 + \mu^2).
\]

An atomic form factor \(F(q, Z)\), which accounts for the overall effect of the electron charge
Figure 2.7: Coherent (Rayleigh) scattering process [80]

distribution of the target nuclei that the photon experiences as it collides with the bound outer shell electron, is applied to the Thomson scattering DCS to yield the Rayleigh scattering DCS:

$$\frac{d\sigma_{co}}{d\Omega} = \frac{d\sigma_T}{d\Omega} [F(q, Z)]^2, \quad (2.43)$$

where $F(q, Z)$ is dependent on the recoil momentum $q$, and the atomic number $Z$ of the background material. The atomic form factor can approximated based on the atomic model of Hartree-Fock. Some notable calculations have been performed by Hubbell et al. [35, 36], Doyle and Turner [21], and Cromer and Liberman [18].

2.2.3 Incoherent (Compton) Scattering

Incoherent scattering, or Compton scattering, is the most frequently occurring photon interaction and is dominant in the mid-energy regime as well as the low and high energy regime for low $Z$ materials. This phenomenon, depicted in Figure 2.8, involves the collision of an incident photon of energy $E = hv$ on a loosely bound electron, often approximated as a free electron at rest. This collision results in the absorption of the incident photon energy by the electron, which is then ejected with an outgoing energy $E_e$ and direction $\theta_e$. The remaining energy is conserved by a scattered secondary photon with an outgoing energy
$E'$ and direction $\theta$. Using the conservation of energy and momentum yields the following system of equations, which provides the relationship between the incident photon energy $E$, the outgoing electron energy $E_e$ and scattering cosine $\mu_e = \cos \theta_e$, and the secondary photon energy $E'$ and scattering cosine $\mu = \cos \theta$ [97]:

\[
E' = \frac{E}{1 + \kappa (1 - \mu)}, \tag{2.44}
\]

\[
E_e = \frac{E}{1 + \kappa (1 - \mu_e)}, \tag{2.45}
\]

\[
\frac{1}{\tan \theta} = (1 + \kappa) \tan \frac{\theta_e}{2}. \tag{2.46}
\]

To solve this system of equations, the scattering angle of the outgoing photon must be sampled from the Compton scattering DCS, which is expressed using the Klein-Nishina distribution [43] for a free electron:

\[
\frac{d\sigma_{KN}}{d\Omega} = \frac{r_e^2}{2} \left( \frac{\lambda}{\lambda'} \right)^2 \left[ \frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - (1 - \mu^2) \right], \tag{2.47}
\]

\[
\frac{\lambda}{\lambda'} = \frac{1}{1 + \kappa (1 - \mu)}. \tag{2.48}
\]

This expression was derived using the Dirac equation [20], which accounts for the quantum mechanical nature of the free electron. It is typically sampled using Kahn’s rejection scheme [38] for $E < 1.4$ MeV and Koblinger’s rejection scheme [44] for $E \geq 1.4$ MeV. We
note that as the incident photon approaches low energies, \( \frac{E'}{E} \to 1 \), Thomson scattering is recovered. In the case when the target electron cannot be approximated as a free electron, the Klein-Nishina distribution must be modified with the form factor \( S(q, Z) \):

\[
\frac{d\sigma_{\text{KN}}^{\text{in}}}{d\Omega} = \frac{r_e^2}{2} \left( \frac{\lambda}{\lambda'} \right)^2 \left[ \frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - (1 - \mu^2) \right] S(q, Z),
\]

which accounts for the Doppler broadening that occurs in the scattered photon as a result of the incident photon colliding with a moving electron.

### 2.2.4 Electron-Positron Pair Production

Electron-positron pair production is a photon interaction that is dominant at high energies, and the model explicitly accounts for energy, momentum, and electric charge conservation. During this process, shown in Figure 2.9, a photon of energy \( E \) interacts with and destabilizes a target nuclei assumed to have infinite mass. If the photon is energetic enough, \( 2m_e c^2 \) of its kinetic energy is converted into mass and an electron-positron pair is produced. The remaining photon energy \( E_+ + E_- = E - 2m_e c^2 \) is imparted on the electron-positron pair in the form of kinetic energy. Because energy must be conserved, this interaction is only energetically allowed for photon energies \( E \geq 2m_e c^2 \). The energies of the electron and

![Figure 2.9: Electron-positron pair production process [80]](attachment:image)
The positron are computed using conservation of energy:

\[
E_- = \epsilon E - m_e c^2, \quad (2.50)
\]

\[
E_+ = E - E_- - 2m_e c^2, \quad (2.51)
\]

where \(\epsilon\) is the energy fraction transferred to the electron. On average, the energy fraction transferred is half of the photon energy. It can be sampled using the pair production DCS, expressed as [80]

\[
\frac{d\sigma_{pp}}{d\epsilon} = r_\epsilon^2 \alpha Z [Z + \eta] \left\{ [\epsilon^2 + (1 - \epsilon)^2](\varphi_1 - 4f_C) + \frac{2}{3} \epsilon(1 - \epsilon)(\varphi_2 - 4f_C) \right\}, \quad (2.52)
\]

where \(\eta\) considers triplet production [34], \(\varphi_1\) and \(\varphi_2\) are screening functions expressed by Tsai [94, 95], and \(f_C\) is a Coulomb correction function expressed by Davies et al. [19]. The angular distribution [33, 65], normalized by constant \(a\), of the electron and positron is

\[
p(\mu_\pm) = \frac{a}{\sqrt{1 - \beta_\pm \mu_\pm}}, \quad (2.53)
\]

\[
\mu_\pm = \cos \theta_\pm. \quad (2.54)
\]

The positron produced is transported similar to an electron. However, unlike an electron, which deposits energy at \(E < 1\) keV, a positron annihilates at \(E < 1\) keV and produces two photons, as discussed in Section 2.1.4.

### 2.3 Coupled Photon-Electron Transport

As photons, electrons, and positrons move through a medium, the production of secondary particles from interactions described in Sections 2.1 and 2.2 can be represented with the time-dependent, linearized Boltzmann transport equation, which is valid for describing single-scatter photon-electron transport. We first define the following photon quantities with
superscript $\gamma$ and consider photoelectric absorption, Compton scattering, and pair production interactions:

$$\psi_{\gamma}(x, \hat{\Omega}, E, t) = \text{Angular flux of photons},$$

$$\Sigma_{\gamma}^t(x, E) = \text{Total photon interaction cross section},$$

$$\Sigma_{\gamma}^{pe}(x, E) = \text{Photoelectric photon interaction cross section},$$

$$\Sigma_{\gamma}^{pp}(x, E) = \text{Pair production photon interaction cross section},$$

$$\Sigma_{\gamma}^s(x, \hat{\Omega} \cdot \hat{\Omega}', E' \rightarrow E) = \text{Double-differential photon Compton scattering cross section},$$

$$\chi_{br,e^-}^\gamma(x, \hat{\Omega} \cdot \hat{\Omega}, E' \rightarrow E) = \text{Photon spectrum of electron-bremsstrahlung collisions},$$

$$\chi_{br,e^+}^\gamma(x, \hat{\Omega} \cdot \hat{\Omega}, E' \rightarrow E) = \text{Photon spectrum of positron-bremsstrahlung collisions},$$

$$\nu_{br}^- (x, E) = \text{Mean number of photons emitted per bremsstrahlung collision},$$

$$Q_{\gamma}(x, \hat{\Omega}, E, t) = \text{Internal photon source}.$$

Electron quantities are defined with superscript $e^-$ and consider bremsstrahlung emission and inelastic scattering interactions:

$$\psi_{e^-}(x, \hat{\Omega}, E, t) = \text{Angular flux of electrons},$$

$$v_{e^-} (E) = \text{Speed of electron},$$

$$\Sigma_{e^-}^t(x, E) = \text{Total electron interaction cross section},$$

$$\Sigma_{br}^{e^-}(x, E) = \text{Bremsstrahlung emission electron interaction cross section},$$

$$\Sigma_{e^+_g}^{-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) = \text{Double-differential electron inelastic scattering cross section},$$

$$\chi_{pe}^{-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) = \text{Electron spectrum of photon photoelectric interaction},$$

$$\chi_{s,\gamma}^{-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) = \text{Electron spectrum of photon Compton collisions},$$

$$\chi_{pe}^{e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) = \text{Electron spectrum of photon pair production interaction},$$

$$Q_{e^-}(x, \hat{\Omega}, E, t) = \text{Internal electron source}. $$
Finally, positron quantities are defined with superscript $e^+$ and consider bremsstrahlung emission, inelastic scattering, and positron annihilation interactions:

$$\psi_e^+(x, \hat{\Omega}, E, t) = \text{Angular flux of positrons},$$
$$v_e^+(E) = \text{Speed of positron},$$
$$\Sigma_i^e(x, E) = \text{Total positron interaction cross section},$$
$$\Sigma_{br}^e(x, E) = \text{Bremsstrahlung emission positron interaction cross section},$$
$$\Sigma_{an}^e(x, E) = \text{Annihilation positron interaction cross section},$$
$$\Sigma_s^e(x, \hat{\Omega}', \hat{\Omega}, E' \rightarrow E) = \text{Double-differential positron inelastic scattering cross section},$$
$$\chi_{pe}^e(x, \hat{\Omega}', \hat{\Omega}, E' \rightarrow E) = \text{Positron spectrum of photon pair production interaction},$$
$$Q^e(x, \hat{\Omega}, E, t) = \text{Internal positron source},$$

where $x = \langle x, y, z \rangle$ is the spatial coordinate, $\hat{\Omega} = \langle \mu, \phi \rangle$ is the directional unit vector, $\mu = \cos \theta \in [-1, 1]$ is the polar cosine, $\phi \in [0, 2\pi]$ is the azimuthal angle, $E$ is the kinetic energy of the particle, and $t$ is time.

The photon, electron, and positron (for completeness) time-dependent, linearized Boltzmann transport equations and boundary conditions, respectively, can be formulated by the conservation of particles, which enforce that the rate of change in the number of particles is
equal to the rate of particles gained minus the rate of particles lost:

\[
\frac{1}{c} \frac{\partial \psi^\gamma}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi^\gamma(x, \hat{\Omega}, E, t) + \Sigma_t^\gamma(x, E) \psi^\gamma(x, \hat{\Omega}, E, t)
\]
\[
= \int_0^\infty \int_0^{4\pi} \Sigma_a^\gamma(x, \hat{\Omega} \cdot \hat{\Omega}, E', \psi^\gamma(x, \hat{\Omega}, E, t) d\Omega' dE'
\]
\[
+ \frac{2\delta(E - m_e c^2)}{4\pi} \int_0^\infty \int_0^{4\pi} \Sigma_{an}^e(x, E') \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE'
\]
\[
+ \int_0^{4\pi} \int_0^\infty \chi_{br,e^+}(x, \hat{\Omega}' \cdot \hat{\Omega}, E', \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE'
\]
\[
+ \int_0^{4\pi} \int_0^\infty \chi_{br,e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E', \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE'
\]
\[
+ Q^\gamma(x, \hat{\Omega}, E, t),
\]

\[\text{(2.55a)}\]

\[
\frac{1}{v_e^-(E)} \frac{\partial \psi^e^-}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi^e^- (x, \hat{\Omega}, E, t) + \Sigma_t^e(x, E) \psi^e^- (x, \hat{\Omega}, E, t)
\]
\[
= \int_0^\infty \int_0^{4\pi} \Sigma_a^e(x, \hat{\Omega} \cdot \hat{\Omega}, E', \psi^e^-(x, \hat{\Omega}, E', t) d\Omega' dE'
\]
\[
+ \int_0^{4\pi} \int_0^\infty \chi_{pe,e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E', \psi^e^-(x, \hat{\Omega}, E', t) d\Omega' dE'
\]
\[
+ \int_0^{4\pi} \int_0^\infty \chi_{s,\gamma,e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E', \psi^e^-(x, \hat{\Omega}, E', t) d\Omega' dE'
\]
\[
+ \int_0^{4\pi} \int_0^\infty \chi_{pp,e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E', \psi^e^-(x, \hat{\Omega}, E', t) d\Omega' dE'
\]
\[
+ Q^e^-(x, \hat{\Omega}, E, t),
\]

\[\text{(2.55b)}\]
\[
\frac{1}{\nu^e(E)} \frac{\partial \psi^e}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi^e(x, \hat{\Omega}, E, t) + \Sigma^e_i(x, E) \psi^e(x, \hat{\Omega}, E, t)
= \int_0^\infty \int_{4\pi} \Sigma^e_{an}(x, E') \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE' \\
+ \int_0^\infty \int_{4\pi} \chi_{pp}^\gamma(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \Sigma_{pp}^\gamma(x, E') \psi^\gamma(x, \hat{\Omega}, E', t) d\Omega' dE' \\
+ Q^e(x, \hat{\Omega}, E, t),
\] (2.55c)

\[
\psi^\gamma(x, \hat{\Omega}, E, t) = \psi^b(x, \hat{\Omega}, E, t), \quad x \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0, \quad 0 < E < \infty, \quad 0 < t,
\] (2.55d)

\[
\psi^e^-(x, \hat{\Omega}, E, t) = \psi^b(x, \hat{\Omega}, E, t), \quad x \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0, \quad 0 < E < \infty, \quad 0 < t,
\] (2.55e)

\[
\psi^e^+(x, \hat{\Omega}, E, t) = \psi^b(x, \hat{\Omega}, E, t), \quad x \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0, \quad 0 < E < \infty, \quad 0 < t.
\] (2.55f)

The first term on the left-hand side of each of these transport equations, Eqs (2.55a), (2.55b), and (2.55c), is the rate of change term in the number of particles. The second and third terms on the left-hand side of each of these transport equations represent the rate of particles lost due to leakage and collisions, respectively. The first and last terms on the right-hand side of each of these equations are the scattering source and internal source, respectively.

In Eq. (2.55a), the coupling terms are

\[
\frac{2\delta(E - m_e c^2)}{4\pi} \int_0^\infty \int_{4\pi} \Sigma^e_{an}(x, E') \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE',
\] (2.56)

\[
\int_0^\infty \int_{4\pi} \chi^\gamma_{br,e^+}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \nu^\gamma(x, E) \Sigma^e_{br}(x, E') \psi^e(x, \hat{\Omega}, E, t) d\Omega' dE',
\] (2.57)

\[
\int_0^\infty \int_{4\pi} \chi^\gamma_{br,e^-}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \nu^\gamma(x, E) \Sigma^e_{br}(x, E') \psi^e^-(x, \hat{\Omega}, E, t) d\Omega' dE',
\] (2.58)

where these expressions describe the production of exactly two photons from positron annihilation at the electron rest mass energy \(m_e c^2\) isotropically, and bremsstrahlung emission
from positrons and electrons, respectively. In Eq. (2.55b), the coupling terms are

\[
\int_0^\infty \int_0^{4\pi} \chi_{pe}^e(x, \hat{\Omega}, E) \Sigma_{pe}^\gamma(x, \hat{\Omega}, E', t) d\hat{\Omega} dE',
\]

\[
\int_0^\infty \int_0^{4\pi} \chi_{s,\gamma}^e(x, \hat{\Omega}, E) \Sigma_{s}^\gamma(x, \hat{\Omega}, E', t) d\hat{\Omega} dE',
\]

\[
\int_0^\infty \int_0^{4\pi} \chi_{pp}^e(x, \hat{\Omega}, E) \Sigma_{pp}^\gamma(x, \hat{\Omega}, E', t) d\hat{\Omega} dE',
\]

where these expressions describe the production of electrons from photon photoelectric effect, Compton scattering, and pair production, respectively. In Eq. (2.55c), the coupling term is

\[
\int_0^\infty \int_0^{4\pi} \chi_{pp}^e(x, \hat{\Omega}, E) \Sigma_{pp}^\gamma(x, \hat{\Omega}, E', t) d\hat{\Omega} dE',
\]

which describes the production of a positron via photon pair production.

### 2.3.1 Simulation Techniques

The particles described by this set of equations can be simulated using the computationally expensive single-scatter Monte Carlo approach, in which a particle history is initialized by randomly sampling a source particle’s initial energy, position, and direction of flight. Depending on the material properties the particle is currently in and its energy state, its distance to particle interaction is sampled to determine the particle’s next position and interaction type. In the event that the particle scatters, a new direction of flight is sampled based on the distribution of scattering angles, and a new energy is sampled based on the kinematics of the event. For photons, this random walk is repeated until the particle is absorbed or leaks from the system. For electrons, the random walk ends once its energy falls below a specified threshold or leaks, and for positrons, the random walk ends once it annihilates or leaks.
To solve these equations deterministically using the $P_N$ method, the scattering term is typically expanded using the spherical harmonics functions and Legendre polynomials. This expansion begins by expanding the differential scattering cross section in Legendre polynomials

$$
\Sigma_s(x, \Omega', \Omega, E' \rightarrow E, t) = \sum_{k=0}^{\infty} \left( \frac{2k + 1}{4\pi} \right) \Sigma_{s,k}(x, E' \rightarrow E, t) P_k(\Omega' \cdot \Omega),
$$

(2.63)

$$
\Sigma_{s,k}(x, E' \rightarrow E, t) = 2\pi \int_{-1}^{1} P_k(\mu) \Sigma_s(x, \mu, E' \rightarrow E, t) d\mu,
$$

(2.64)

and expanding the angular flux in spherical harmonics

$$
\psi(x, \hat{\Omega}', E', t) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \psi_{n,m}(x, E', t) Y_n^m(\hat{\Omega}'),
$$

(2.65)

$$
\psi_{n,m}(x, E', t) = \int_{4\pi} \psi(x, \hat{\Omega}', E', t) Y_n^{-m}(\hat{\Omega}') d\Omega'.
$$

(2.66)

Combining Eqs. (2.63) and (2.65) and rearranging terms, the scattering term becomes

$$
\int_{4\pi} \Sigma_s(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \psi(x, \hat{\Omega}', E', t) d\Omega'
$$

$$
= \int_{4\pi} \left[ \sum_{k=0}^{\infty} \left( \frac{2k + 1}{4\pi} \right) \Sigma_{s,k}(x, E' \rightarrow E, t) P_k(\hat{\Omega}' \cdot \hat{\Omega}) \right] \times \left[ \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \psi_{n,m}(x, E', t) Y_n^m(\hat{\Omega}') \right] d\Omega'
$$

$$
= \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left( \frac{2k + 1}{4\pi} \right) \Sigma_{s,k}(x, E' \rightarrow E, t) \psi_{n,m}(x, E', t) \int_{4\pi} P_k(\hat{\Omega}' \cdot \hat{\Omega}) Y_n^m(\hat{\Omega}') d\Omega'
$$

$$
= \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left( \frac{2k + 1}{4\pi} \right) \Sigma_{s,k}(x, E' \rightarrow E, t) \psi_{n,m}(x, E', t) \times J_{k,n,m},
$$

(2.67)

$$
J_{k,n,m} = \int_{4\pi} P_k(\hat{\Omega}' \cdot \hat{\Omega}) Y_n^m(\hat{\Omega}') d\Omega'.
$$

(2.68)
Using the addition formula for Legendre polynomials and the orthogonality condition of spherical harmonics, Eq. (2.68) can be reduced to

\[
J = \int_{4\pi} P_k(\hat{\Omega} \cdot \hat{\Omega}') Y_n^m(\hat{\Omega}') d\Omega'
\]

\[
= \int_{4\pi} \left[ \frac{4\pi}{2k+1} \sum_{l=-k}^k Y_k^l(\hat{\Omega}) Y_{k-l}^-(\hat{\Omega}') \right] Y_n^m(\hat{\Omega}') d\Omega'
\]

\[
= \frac{4\pi}{2k+1} \sum_{l=-k}^k Y_k^l(\hat{\Omega}) \int_{4\pi} Y_{k-l}^-(\hat{\Omega}') Y_n^m(\hat{\Omega}') d\Omega'
\]

\[
= \frac{4\pi}{2k+1} \sum_{l=-k}^k Y_k^l(\hat{\Omega}) \delta_{n,k} \delta_{l,m}
\]

\[
= \frac{4\pi}{2k+1} Y_k^m(\hat{\Omega}) \delta_{n,k}.
\] (2.69)

Inserting this result into Eq. (2.67) and applying Eq. (2.64) yields

\[
\int_{4\pi} \Sigma_s(x, \hat{\Omega} \cdot \hat{\Omega}, E' \rightarrow E) \psi(x, \hat{\Omega}', E', t) d\Omega'
\]

\[
= \sum_{k=0}^\infty \sum_{n=0}^\infty \sum_{m=-n}^n \left( \frac{2k+1}{4\pi} \right) \Sigma_{s,k}(x, E' \rightarrow E, t) \psi_{n,m}(x, E', t) \left[ \frac{4\pi}{2k+1} Y_k^m(\hat{\Omega}) \right]
\]

\[
= \sum_{n=0}^\infty \sum_{m=-n}^n \Sigma_{s,n}(x, E' \rightarrow E, t) \psi_{n,m}(x, E', t) Y_n^m(\hat{\Omega})
\]

\[
= \sum_{n=0}^\infty \sum_{m=-n}^n \left[ 2\pi \int_{-1}^1 P_n(\mu) \Sigma_s(x, \mu, E' \rightarrow E, t) d\mu \right] \psi_{n,m}(x, E', t) Y_n^m(\hat{\Omega}).
\] (2.70)
Inserting this expression into the electron linear Boltzmann transport equation, Eq. (2.55b), results in the equivalent formulation

\[
\frac{1}{v^e(E)} \frac{\partial \psi^e(x, \hat{\Omega}, E, t)}{\partial t} + \hat{\Omega} \cdot \nabla \psi^e(x, \hat{\Omega}, E, t) + \Sigma_i^e(x, E) \psi^e(x, \hat{\Omega}, E, t)
\]

\[
= 2\pi \sum_{n=0}^{\infty} \sum_{m=-n}^{n} Y_n^m(\hat{\Omega}) \int_0^{\infty} \psi^e_{n,m}(x, E', t) \int_{-1}^{1} P_n(\mu) \Sigma_n^e(x, \mu, E' \rightarrow E, t) d\mu dE
\]

\[
+ \int_0^{\infty} \int_0^{4\pi} \chi_{pe}^e(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \Sigma_{pe}(x, E') \psi^\gamma(x, \hat{\Omega}, E', t) d\Omega' dE'
\]

\[
+ \int_0^{\infty} \int_0^{4\pi} \chi_{s,\gamma}^e(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \Sigma_s^\gamma(x, E') \psi^\gamma(x, \hat{\Omega}, E', t) d\Omega' dE'
\]

\[
+ \int_0^{\infty} \int_0^{4\pi} \chi_{pp}^e(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \Sigma_{pp}(x, E') \psi^\gamma(x, \hat{\Omega}, E', t) d\Omega' dE'
\]

\[
+ Q^e(x, \hat{\Omega}, E, t).
\]

(2.71)

In practice, the expanded scattering term is truncated at a low order for practical computing purposes and can achieve a high degree of accuracy when the particle is assumed to experience nearly isotropic scattering. However, this assumption cannot be applied to electron transport because the scattering of soft collisions are so forward-peaked and would require a large number of expansion terms to accurately capture the scattering behavior, making it impractical to compute, which motivates the development of the Boltzmann-Fokker-Planck equation.

2.3.2 Boltzmann-Fokker-Planck Equation

The Boltzmann-Fokker-Planck (BFP) equation can be derived from the time-dependent, linearized Boltzmann transport equation for electrons, Eq. (2.71), by assuming that, as the electron travels through a medium, the energy loss rate of the electron is fixed between hard collisions such that the scattering kernel is not highly peaked. This equation is valid for
electron transport problems that are dominant with soft collisions, in which the electron experiences small changes in direction and energy except for the infrequent hard collision, which results in a larger change in electron direction and energy.

To derive the BFP equation from the electron time-dependent, linearized Boltzmann transport equation, we begin by lumping the photon coupling terms into the inhomogeneous source term for brevity:

\[
\frac{1}{v^e(E)} \frac{\partial \psi^e}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi^e(x, \hat{\Omega}, E, t) + \Sigma^e_t(x, E) \psi^e(x, \hat{\Omega}, E, t)
\]

\[
= 2\pi \sum_{n=0}^{\infty} \sum_{m=-n}^{n} Y^m_n(\hat{\Omega}) \int_0^\infty \psi^e_{n,m}(x, E', t) \int_{-1}^{1} P_n(\mu) \Sigma^e_n(x, \mu, E' \rightarrow E, t) d\mu dE
\]

\[
+ Q^e(x, \hat{\Omega}, E, t). \quad (2.72)
\]

We then express the electron differential scattering cross section as the sum of the electron differential scattering cross section for hard collisions and soft collisions:

\[
\Sigma^e_s(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t) = \Sigma^e_{s,h}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t) + \Sigma^e_{s,s}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t), \quad (2.73)
\]

\[
\Sigma^e_s(x, E, t) = \Sigma^e_{s,h}(x, E, t) + \Sigma^e_{s,s}(x, E, t), \quad (2.74)
\]

where

\[
\Sigma^e_{s,h}(x, E, t) = \int_0^{\infty} \int_{4\pi}^{\infty} \Sigma^e_{s,h}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t) d\Omega' dE', \quad (2.75)
\]

\[
\Sigma^e_{s,s}(x, E, t) = \int_0^{\infty} \int_{4\pi}^{\infty} \Sigma^e_{s,s}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t) d\Omega' dE', \quad (2.76)
\]

\[
\Sigma^e_{s,s}(x, E, t) = \int_0^{\infty} \int_{4\pi}^{\infty} \Sigma^e_{s,s}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E, t) d\Omega' dE'. \quad (2.77)
\]

We note that hard collisions result in large direction and energy changes while soft collisions are highly peaked, and \(\Sigma^e_{s,s}(x, \hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E)\) is large for \(\hat{\Omega}' \cdot \hat{\Omega} \rightarrow 1\) and energy losses are
small such that $E \approx E'$. Applying these terms to Eq. (2.72) yields

$$
\frac{1}{v_e(E)} \frac{\partial \psi_e^-}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi_e^- (x, \hat{\Omega}, E, t) + \left[ \Sigma_t^- (x, E, t) - \Sigma_{s,s}^- (x, E, t) \right] \psi_e^- (x, \hat{\Omega}, E, t)
$$

$$+ \Sigma_{s,s}^- (x, E, t) \psi_e^- (x, \hat{\Omega}, E, t) = \int_0^\infty \int_{4\pi}^\infty \Sigma_{s,h}^- (x, \hat{\Omega}, E') \psi_e^- (x, \hat{\Omega}, E' \rightarrow E, t) d\Omega' dE'
$$

$$- \int_0^\infty \int_{4\pi}^\infty \Sigma_{s,s}^- (x, \hat{\Omega}', \hat{\Omega}, E' \rightarrow E, t) \psi_e^- (x, \hat{\Omega}', E', t) d\Omega' dE'
$$

$$+ Q_e^- (x, \hat{\Omega}, E, t). \quad (2.78)
$$

Rearranging terms and collecting soft scattering terms gives the expression

$$
\frac{1}{v_e^-} \frac{\partial \psi_e^-}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi_e^- (x, \hat{\Omega}, E, t) + \left[ \Sigma_t^- (x, E, t) - \Sigma_{s,s}^- (x, E, t) \right] \psi_e^- (x, \hat{\Omega}, E, t)
$$

$$= \int_0^\infty \int_0^\infty \int_0^\infty \Sigma_{s,h}^- (x, \hat{\Omega}', \hat{\Omega}, E') \psi_e^- (x, \hat{\Omega}', E' \rightarrow E, t) d\Omega' dE'
$$

$$+ \int_0^\infty \int_0^\infty \Sigma_{s,s}^- (x, \hat{\Omega}', \hat{\Omega}, E' \rightarrow E, t) \psi_e^- (x, \hat{\Omega}', E', t) d\Omega' dE' - \Sigma_{s,s}^- (x, E) \psi_e^- (x, \hat{\Omega}, E, t)
$$

$$+ Q_e^- (x, \hat{\Omega}, E, t), \quad (2.79a)
$$

$$
\frac{1}{v_e^-} \frac{\partial \psi_e^-}{\partial t}(x, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi_e^- (x, \hat{\Omega}, E, t) + \left[ \Sigma_t^- (x, E, t) - \Sigma_{s,s}^- (x, E, t) \right] \psi_e^- (x, \hat{\Omega}, E, t)
$$

$$= \int_0^\infty \int_0^\infty \int_0^\infty \Sigma_{s,h}^- (x, \hat{\Omega}', \hat{\Omega}, E') \psi_e^- (x, \hat{\Omega}', E' \rightarrow E, t) d\Omega' dE'
$$

$$+ \int_0^\infty \int_0^\infty \Sigma_{s,s}^- (x, \hat{\Omega}', \hat{\Omega}, E' \rightarrow E, t) \psi_e^- (x, \hat{\Omega}', E', t)
$$

$$+ L_{s,s} \psi_e^- (x, \hat{\Omega}', E', t) + Q_e^- (x, \hat{\Omega}, E, t), \quad (2.79b)
$$

where $L_{s,s}$ is the electron soft collision operator. This operator has been shown by Pomeranin [72] to be approximately the Fokker-Planck operator when assuming a smoothly and
continuously changing direction and energy loss from soft collisions and takes the form

\[ L_{s,s} \psi_e^- (x, \hat{\Omega}, E, t) = \]

\[ \int_0^\infty \int_{4\pi} \Sigma_{s,h}^e (x, \hat{\Omega}', \hat{\Omega}', E' \rightarrow E, t) \psi_e^- (x, \hat{\Omega}', E', t) d\Omega' dE' - \Sigma_{s,s}^e (x, E, t) \psi_e^- (x, \hat{\Omega}, E, t), \]

\[ \approx \frac{\Sigma_{s,s, tr}^e (x, E, t)}{2} \left[ \frac{\partial}{\partial \mu} (1 - \mu^2) + \frac{1}{1 - \mu^2} \frac{\partial^2}{\partial \phi^2} \right] \psi_e^- (x, \hat{\Omega}, E, t) + \frac{\partial}{\partial E} S(x, E, t) \psi_e^- (x, \hat{\Omega}, E, t), \]

(2.80)

where \( \Sigma_{s,s, tr}^e (x, E, t) \) is the soft collision transport cross section and \( S(x, E, t) \) is the stopping power. Inserting this term in Eq. (2.79b) results in the Boltzmann Fokker-Planck equation for electrons:

\[ \frac{1}{v_e^- (E)} \frac{\partial \psi_e^- (x, \hat{\Omega}, E, t)}{\partial t} + \hat{\Omega} \cdot \nabla \psi_e^- (x, \hat{\Omega}, E, t) + \left[ \Sigma_t^e (x, E, t) - \Sigma_{s,s}^e (x, E, t) \right] \psi_e^- (x, \hat{\Omega}, E, t) \]

\[ = \int_0^\infty \int_{4\pi} \Sigma_{s,h}^e (x, \hat{\Omega}', \hat{\Omega}', E' \rightarrow E, t) \psi_e^- (x, \hat{\Omega}', E', t) d\Omega' dE' \]

\[ + \frac{\Sigma_{s,s, tr}^e (x, E, t)}{2} \left[ \frac{\partial}{\partial \mu} (1 - \mu^2) + \frac{1}{1 - \mu^2} \frac{\partial^2}{\partial \phi^2} \right] \psi_e^- (x, \hat{\Omega}, E, t) \]

\[ + \frac{\partial}{\partial E} S(x, E, t) \psi_e^- (x, \hat{\Omega}, E, t) + Q_e^- (x, \hat{\Omega}, E, t). \]

(2.81)

The BFP equation can be solved using a Monte Carlo approach similar to the condensed history algorithm. Though, the BFP equation is typically solved using a deterministic approach [63].
Simulating single-scatter electron interactions can be computationally expensive and impractical for routine calculations. To improve computation time while preserving accuracy, multiple scattering theories have been developed to compute the overall angular deflection and energy loss distributions of an electron for multiple interactions that may occur within some pathlength traversed in a uniform background material. These theories have been incorporated into Monte Carlo condensed history algorithms in which the history of an electron is “condensed” into steps that represent multiple electron interactions. This chapter discusses the multi-scatter theories used in current condensed history methods for uniform background materials and reviews the Class I and II condensed history algorithms. In the subsequent chapter (Chapter 4), these methods are extended to account for randomly varying material backgrounds.

3.1 Step Size

For a Class I condensed history algorithm, discussed in more detail in Section 3.5.1, the step length \( s = s_m - s_{m-1} \) of an electron is typically computed assuming an 8.3\% energy loss [109], which is based on empirical studies of the required accuracy and computing
performance:

\[ E_{m-1} - E_m = - \int_{s_{m-1}}^{s_m} \left( \frac{dE}{ds} \right)_{tot} ds, \]  

(3.1)

where \( s_m \) and \( E_m \) are the total path length and electron kinetic energy at the end of \( m \) steps and \( \left( \frac{dE}{ds} \right)_{tot} \) is the total stopping power. The calculation of the multi-scatter distributions for an electron are dependent on its kinetic energy and associated step length. As the kinetic energy of an electron increases, the computed step length generally increases to satisfy the 8.3% energy loss condition. The step lengths of a \( E = 0.1 \) MeV and \( E = 10 \) MeV electron traveling through carbon and lead are provided in Table 3.1.

<table>
<thead>
<tr>
<th>( E ) [MeV]</th>
<th>Step Length [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Carbon</td>
</tr>
<tr>
<td>0.1</td>
<td>( 1.10 \times 10^{-3} )</td>
</tr>
<tr>
<td>10</td>
<td>( 2.06 \times 10^{-1} )</td>
</tr>
</tbody>
</table>

Table 3.1: Step lengths of an electron with kinetic energies 10 MeV and 0.1 MeV when traveling through materials carbon and lead

3.2 Angular Deflection

The multiple-scattering angular deflection distribution can be derived from the conservation of particles scattering in and out of an angular interval with deflection \( \theta' \)

\[ \frac{\partial f}{\partial s}(\theta, s) = -N f(\theta, s) \int_{0}^{\pi} \sigma(\theta') \sin(\theta')d\theta' + N \int_{0}^{\pi} f(\theta - \theta', s) \sigma(\theta') \sin(\theta')d\theta', \]  

(3.2)

where \( \theta \) is the deflection angle of the electron after traveling a distance \( s \) through a material of atomic number density \( N \) and \( \sigma(\theta') \sin(\theta')d\theta' \) is the probability of a single scatter at an angle \( \theta' \) into \( d\theta' \). To solve this problem, Molière first used a small-angle approximation \( \theta \ll 1 \)
such that \( \sin(\theta') \approx \theta' \), which resulted in an expression in the \( \theta \)-plane \[61\]:

\[
\frac{\partial f}{\partial s}(\theta, s) = -N f(\theta, s) \int_0^\pi \sigma(\theta') \theta' d\theta' + N \int_0^\pi f(\theta - \theta', s) \sigma(\theta') \theta' d\theta'.
\]

(3.3)

Molière then applied a Bessel transformation to obtain the final result:

\[
f(\theta, s) = \int_0^\infty k J_0(k \theta) \exp \left\{ -Ns \int_0^\pi \sigma(\theta') \theta' \left[ 1 - J_0(k \theta') \right] d\theta' \right\} dk,
\]

(3.4)

where \( k \) is the number of scatters and \( J_0(x) \) is a Bessel function of the first kind, Eq. (2.11b). Because of the small-angle approximation, this theory is best suited for smaller step lengths to maintain accuracy and breaks down for larger step sizes because they may result in larger angular deflections that are not adequately captured by this distribution.

Goudsmit and Saunderson derived a more robust angular deflection distribution that is exact and not limited to small scattering angles, which is used in this work and is described in more detail in Section 3.2.1 \[30\]. Subsequently, Lewis derived a multi-scatter angular deflection distribution with the intent of acquiring an exact result beginning with the expression \[56\]

\[
\frac{\partial f}{\partial s}(x, \hat{\Omega}, s) + \hat{\Omega} \cdot \nabla f(x, \hat{\Omega}, s) = N \int_{4\pi} \left[ f(x, \hat{\Omega}', s) - f(x, \hat{\Omega}, s) \right] \sigma_s \left( \hat{\Omega}' \cdot \hat{\Omega} \right) d\Omega',
\]

(3.5)

where \( f(x, \hat{\Omega}, s) \) is the angular deflection distribution and \( N \) is the atomic number density. Lewis solved this using spherical harmonics and integrating over position \( x \), which resulted in a solution that agreed with the angular deflection distribution of Goudsmit and Saunderson:

\[
F(s, \mu) = \sum_{l=0}^\infty \left( l + \frac{1}{2} \right) G_l(s) P_l(\mu),
\]

(3.6)

\[
G_l(s) = \exp \left\{ -2\pi N s \int_{-1}^1 \frac{d\sigma_s^- (\mu)}{d\Omega} [1 - P_l(\mu)] d\mu \right\}.
\]

(3.7)
3.2.1 Goudsmit & Saunderson

The multi-scatter angular deflection distribution derived by Goudsmit and Saunderson is commonly used in standard condensed history algorithms and is used in this work. In this section, we provide a detailed derivation of this distribution.

Goudsmit and Saunderson’s theory relies on a Legendre polynomial expansion \[30\] to exactly compute the overall scattering angle \( \theta \) of an electron after \( k \) scatters in a uniform domain. This multi-scatter angular deflection distribution can be derived beginning with the simplest case of two consecutive, independent scatters, where \( \mu_1 = \cos(\theta_1) \) and \( \mu_2 = \cos(\theta_2) \) are the scattering cosines of the first and second scatter, \( \phi_1 \) and \( \phi_2 \) are the azimuthal angle of the first and second scatter. If \( \mu \) is the overall scattering cosine after both scatters, then the addition theorem of spherical harmonics gives

\[
P_l(\mu) = P_l(\mu_1)P_l(\mu_2) + 2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P^m_l(\mu_1)P^m_l(\mu_2) \cos [m(\phi_1 - \phi_2)].
\] (3.8)

Because the scattering process is azimuthally symmetric, the second term goes to zero when taking the expectation of this expression, which, when accounting for the independence of consecutive scatters, results in the expression

\[
E[P_l(\mu)] = E\left[P_l(\mu_1)P_l(\mu_2) + 2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P^m_l(\mu_1)P^m_l(\mu_2) \cos [m(\phi_1 - \phi_2)]\right] 
= E\left[P_l(\mu_1)P_l(\mu_2)\right] + E\left[2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P^m_l(\mu_1)P^m_l(\mu_2) \cos [m(\phi_1 - \phi_2)]\right] 
= E\left[P_l(\mu_1)P_l(\mu_2)\right] 
= E\left[P_l(\mu_1)\right] E\left[P_l(\mu_2)\right],
\] (3.9)

where \( E[P_l(\mu)] \) is the mean value of the \( \ell^{th} \) order Legendre polynomial. Because scatters are independent processes, it is valid to repetitively take the addition theorem of spherical harmonics for \( k \) scatters, which yields the expectation of the Legendre polynomial to the
For the multi-scatter angular deflection distribution, the mean of all possible number of scatters over some distance traveled must be accounted for in the Legendre expansion coefficient

\[ G_l = \sum_{k=0}^{\infty} W(k) E[P_l(\mu)]^k, \]  

(3.10a)

\[ W(k) = (\Sigma_s^{e^-} s)^k \frac{e^{-\Sigma_s^{e^-} s}}{k!}, \]  

(3.10b)

where \( W(k) \) is the probability of having \( k \) collisions and is a Poisson process because, though scattering events occur randomly, the mean number of scatters \( \Sigma_s^{e^-} s \) is known. Here, \( \Sigma_s^{e^-} = N\sigma_s^{e^-} \) is the electron macroscopic elastic cross section and \( s \) is the distance traveled. Evaluating the Legendre scattering moment using the exponential power series expansion \( e^x = \sum_{n=0}^{\infty} x^n/n! \) reduces to

\[ G_l = \sum_{k=0}^{\infty} W(k) E[P_l(\mu)]^k \]
\[ = \sum_{k=0}^{\infty} (\Sigma_s^{e^-} s)^k \frac{e^{-\Sigma_s^{e^-} s}}{k!} E[P_l(\mu)]^k \]
\[ = \exp \left\{ -\Sigma_s^{e^-} s \right\} \sum_{k=0}^{\infty} \frac{\left\{ \Sigma_s^{e^-} s E[P_l(\mu)] \right\}^k}{k!} \]
\[ = \exp \left\{ -\Sigma_s^{e^-} s \right\} \exp \left\{ \Sigma_s^{e^-} s E[P_l(\mu)] \right\} \]
\[ = \exp \left\{ -\Sigma_s^{e^-} s (1 - E[P_l(\mu)]) \right\} \]
\[ = \exp \left\{ -N\sigma_s^{e^-} s (1 - E[P_l(\mu)]) \right\} \]
\[ = \exp \left\{ -Ns \left( \sigma_s^{e^-} - \sigma_s^{e^-} E[P_l(\mu)] \right) \right\}. \]  

(3.11)
Using the integral of the elastic scattering DCS and relating the expectation of the Legendre polynomial to the Legendre moments of the DCS gives the relationships

\[ \sigma_s^{e^-} = 2\pi \int_{-1}^{1} \frac{d\sigma_s^{e^-}}{d\Omega}(\mu)d\mu, \]  

\[ \sigma_s^{e^-} E[P_l(\mu)] = \sigma_{s,l}^{e^-}, \]  

\[ = 2\pi \int_{-1}^{1} \frac{d\sigma_s^{e^-}}{d\Omega}(\mu)P_l(\mu)d\mu, \]  

with the overall scattering cross section being the first Legendre moment \( \sigma_s^{e^-} = \sigma_{s,0}^{e^-} \). Applying Eqs. (3.12) to Eq. (3.11) gives the final expression of the Legendre scattering moment, which now can be used to express the multi-scatter angular deflection for a uniform background material:

\[ F(s, \mu) = \sum_{l=0}^{\infty} \left( l + \frac{1}{2} \right) G_l(s)P_l(\mu), \]  

\[ G_l(s) = \exp \left\{ -2\pi N s \int_{-1}^{1} \frac{d\sigma_s^{e^-}}{d\Omega}(\mu) [1 - P_l(\mu)]d\mu \right\}, \]  

where \( s \) is the length of the substep, \( \mu = \cos \theta \) is the angular deflection with respect to the \( x \)-axis, \( P_l(\mu) \) is the \( l \)th Legendre polynomial, \( N \) is the atom density of the medium, and \( d\sigma_s^{e^-}(\mu)/d\Omega \) is the elastic scattering DCS of an electron as a function of \( \mu \). This DCS is tabulated for energies ranging from 1 keV to 300 keV [76] and can be computed for higher energies using Eq. 2.13, as described in Section 2.1.1.

These distributions are significantly forward peaked and require an order of \( 10^3 \) Legendre moments to produce resolved distributions. Negreanu et al. proposed using the \( N \)-point Gauss-Legendre quadrature formula [66], which can be used to numerically compute any
definite integral of a function $f(x)$ over the interval $x \in [-1, 1]$, for this computation:

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i),$$  \hspace{1cm} (3.15)$$

where $w_i$ are tabulated quadrature weights, $x_i$ are the associated roots of the $n^{th}$ Legendre polynomial, and $n$ is the number of sample points. For the Legendre scattering moment in Eq. 3.14b, the Gauss-Legendre quadrature takes the form

$$\int_{-1}^{1} \frac{d\sigma_s^e(\mu)}{d\Omega}[1 - P_l(\mu)]d\mu \approx \sum_{i=1}^{n} w_i \frac{d\sigma_s^e(\mu_i)}{d\Omega}[1 - P_l(\mu_i)],$$  \hspace{1cm} (3.16)$$

and enables simultaneous, and thus more efficient, computation of the expansion coefficients required for this multi-scatter angular deflection distribution.

### 3.2.2 Angular Deflection Sampling

To sample from the multi-scatter angular deflection distribution presented in Eq. (3.14), this distribution is first tabulated for discrete scattering angles $\mu \in [-1, 1]$. A random number $\xi \in [0, 1]$ is then sampled such that

$$F(s, \mu_i) < \xi < F(s, \mu_{i+1}),$$  \hspace{1cm} (3.17)$$

where $F(s, \mu_i)$ is the value of the angular deflection distribution at scattering angle $\mu_i$. A piecewise-linear interpolation scheme is then used to compute the scattering angle corresponding to $\xi$:

$$\mu_\xi = \mu_i + (\mu_{i+1} - \mu_i) \frac{\xi - F(s, \mu_i)}{F(s, \mu_{i+1}) - F(s, \mu_i)}.$$  \hspace{1cm} (3.18)$$
3.3 Energy Loss Straggling

High energy electrons traversing a material of some length experience fluctuations in energy loss because of the discrete amounts of energy lost from ionization. These fluctuations are especially broad for thin absorbers such that the electron energy loss is not adequately described by the mean collisional energy loss that derives from the collision stopping power, Eq. (2.33). This section details the energy loss straggling distribution derived by Landau [47] and describes the Gaussian convolution and resulting variance that was conducted by Blunck and Leisegang [7] to improve the accuracy of the distribution based on experimental results obtained by White and Millington [106]. The error analysis by Chechin and Ermilova [17] is discussed as well as the proposed improvement of the variance by Seltzer [85] based on this error analysis.

3.3.1 Landau

High energy electrons experience large fluctuations in energy loss, and this energy loss distribution can be represented by solving a kinetic equation that considers the incremental energy loss $dQ$ for an incremental path length traveled $ds$ assuming that the energy loss is small relative to the electron kinetic energy. This governing kinetic equation balances the change in the probability density $f(s, \Delta)$ of an energy loss $\Delta$ after traveling a distance $s$ to the change in the number of particles that enter and leave a given energy interval with energy loss $Q$:

$$\frac{\partial f(s, \Delta)}{\partial s} = \int_{0}^{\infty} w(Q)[f(s, \Delta - Q) - f(s, \Delta)]dQ,$$

(3.19)

where $w(Q)$ is the probability of an energy loss $Q$ per unit path length after a single collision for an electron kinetic energy $E$ and the solution of this balance equation, $f(s, \Delta)$, is the probability of an electron traveling a length $s$ losing an energy $\Delta$. Because the equation involves difference terms of the form $f(s, \Delta - Q)$ in Eq. (3.19), a Laplace transformation is
applied using the variable transformation $\Delta \to \tau$:

$$\hat{F}(s, \tau) = \int_0^\infty f(s, \Delta)e^{-\tau \Delta} d\Delta, \quad (3.20)$$

$$f(s, \Delta) = \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{i\infty+\sigma} e^{\tau \Delta} \hat{F}(s, \tau) d\tau. \quad (3.21)$$

The general solution $f(s, \Delta)$ is solved for by multiplying both sides of Eq. (3.19) by $e^{-\tau \Delta}$, integrating over $d\Delta$, and applying Eqs. (3.20):

$$e^{-\tau \Delta} \frac{\partial f(s, \Delta)}{\partial s} = e^{-\tau \Delta} \int_0^\infty w(Q)[f(s, \Delta - Q) - f(s, \Delta)] dQ, \quad (3.22)$$

$$\frac{\partial}{\partial s} \int_0^\infty e^{-\tau \Delta} f(s, \Delta) d\Delta = \int_0^\infty e^{-\tau \Delta} \int_0^\infty w(Q)[f(s, \Delta - Q) - f(s, \Delta)] dQ d\Delta, \quad (3.23)$$

$$\frac{\partial}{\partial s} \hat{F}(s, \tau) = \int_0^\infty w(Q) \left\{ \int_0^\infty e^{-\tau \Delta}[f(s, \Delta - Q) - f(s, \Delta)] d\Delta \right\} dQ,$$

$$= \int_0^\infty w(Q) \left[ \hat{F}(s, \tau)e^{-\tau Q} - \hat{F}(s, \tau) d\Delta \right] dQ,$$

$$= -\hat{F}(s, \tau) \int_0^\infty w(Q)(1 - e^{-\tau Q}) dQ. \quad (3.24)$$

Solving this first-order ODE yields

$$\hat{F}(s, \tau) = \exp \left[ -\int_0^\infty w(Q)(1 - e^{-\tau Q}) dQ \right]. \quad (3.25)$$
Inserting Eq. (3.25) into Eq. (3.21) results in the general solution

\[
\begin{align*}
f(s, \Delta) &= \frac{1}{2\pi i} \int_{-i\infty + \sigma}^{i\infty + \sigma} \exp(\tau\Delta) \exp \left[ - \int_{0}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ \right] d\tau, \\
f(s, \Delta) &= \frac{1}{2\pi i} \int_{-i\infty + \sigma}^{i\infty + \sigma} \exp \left[ \tau\Delta - s \int_{0}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ \right] d\tau. \quad (3.26)
\end{align*}
\]

The form of \( w(Q) \) changes depending on energy \( Q \) because of the differing physics that dominate the low and high energy loss regimes. For low energy losses, shell effects must be considered but become negligible for larger energy losses that are much greater than the ionization energy of the atomic electrons. The ranges of significance of Eq. (3.26) are

\[
\begin{align*}
\tau Q_0 &\ll 1, \quad (3.27a) \\
\tau Q_{\text{max}} &\gg 1, \quad (3.27b)
\end{align*}
\]

where \( Q_0 \) is the ionization energy of the atomic electrons and \( Q_{\text{max}} \) is the maximum allowable energy transfer. Let \( Q_1 \gg Q_0 \) such that shell effects are negligible for \( Q > Q_1 \). The integral in the exponent of Eq. (3.26) is evaluated by splitting the integral over \( dQ \) at \( Q = Q_1 \), where the ranges \( Q < Q_1 \) and \( Q > Q_1 \) represent small and large energy losses, respectively. For \( Q < Q_1 \) low energy losses, the exponential term of the expression \( 1 - e^{-\tau Q} \) is approximated using a first-order Taylor series expansion, yielding \( \tau Q \):

\[
\int_{0}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ = \int_{0}^{Q_1} w(Q) \tau Q dQ + \int_{Q_1}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ. \quad (3.28)
\]

For the low energy loss range in the first expression on the right-hand side, Livingston and Bethe derived a well-known expression to account for shell effects. This discussion can
be found on pages 262-263 in Ref. [57]:

\[
\tau Q_1 \int_0^Q w(Q) dQ = \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \ln \left( \frac{Q_1}{Q'} \right),
\]

(3.29a)

\[
\ln(Q') = \ln \left[ \frac{(1 - \beta^2) I^2}{2mv^2} \right] + \beta^2,
\]

(3.29b)

\[
I = I_0 Z.
\]

(3.29c)

For high energy losses, shell effects become negligible, and the mean free path of the electron is governed by Coulomb forces of the background material, which is modeled by the semi-classical process known as Rutherford scattering. For this energy loss region, the expression of \( w(Q) \) is known:

\[
w(Q) = \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \frac{1}{Q^2},
\]

(3.30)

where \( e \) is the charge of an electron, \( m_e \) is the mass of an electron, \( N \) is number density, \( Z \) is atomic number, and \( \beta = v/c \). The second term on the right-hand side of Eq. (3.28) is evaluated by applying a factor of \( 1/\tau \) and using a substitution variable \( z = \tau Q \):

\[
\frac{1}{\tau} \int_{Q_1}^\infty w(Q)(1 - e^{-\tau Q}) dQ = \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \int_{Q_1}^\infty \frac{1 - e^{-\tau Q}}{\tau Q^2} dQ,
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \int_{\tau Q_1}^\infty \frac{1 - e^{-z}}{z^2} dz,
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ \int_{\tau Q_1}^\infty \frac{1}{z^2} dz - \int_{\tau Q_1}^\infty \frac{e^{-z}}{z^2} dz \right],
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ \frac{1}{\tau Q_1} - \int_{\tau Q_1}^\infty \frac{e^{-z}}{z^2} dz \right],
\]

(3.31)

Integration by parts \( \int u dv = uv - \int v du \) is performed on the integral in Eq. (3.31) using
integration variables \( u = e^{-\tau Q} \) and \( dv = \frac{1}{Q^2} dQ \):

\[
\int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z^2} dz = \frac{e^{-\tau Q_1}}{\tau Q_1} - \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz. \tag{3.32}
\]

Substituting Eq. (3.32) in Eq. (3.31), using a first-order Taylor Series expansion \( e^{-\tau Q_1} \approx 1 - \tau Q_1 \) (because \( \tau Q_1 \ll 1 \)), and splitting integrals yields

\[
\frac{1}{\tau} \int_{Q_1}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ = \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ \frac{1}{\tau Q_1} - \left( \frac{e^{-\tau Q_1}}{\tau Q_1} - \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz \right) \right],
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ \frac{1 - e^{-\tau Q_1}}{\tau Q_1} + \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz \right],
\]

\[
\approx \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ 1 + \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz \right],
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ 1 + \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz + \int_{0}^{1} \frac{e^{-z}}{z} dz \right],
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ 1 + \int_{\tau Q_1}^{\infty} \frac{1}{z} dz + \int_{\tau Q_1}^{\infty} \frac{e^{-z}}{z} dz + \int_{1}^{\infty} \frac{e^{-z}}{z} dz \right]. \tag{3.33}
\]

Since \( \tau Q_1 \ll 1 \) is assumed in Eq. (3.27), the limits of integration for the second integral of Eq. (3.33) extend from \( z \in [\tau Q_1, 1] \) to \( z \in [0, 1] \). The sum of the second and third integral in Eq. (3.33) is a known expression equal to \(-\gamma \approx -0.577\), where \( \gamma \) is Euler’s Constant, which is defined as the limiting difference between a harmonic series and natural logarithm:

\[
\frac{1}{\tau} \int_{Q_1}^{\infty} w(Q)(1 - e^{-\tau Q}) dQ \approx \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} \left[ 1 + \int_{\tau Q_1}^{\infty} \frac{1}{z} dz + \int_{0}^{1} \frac{e^{-z} - 1}{z} dz + \int_{1}^{\infty} \frac{e^{-z}}{z} dz \right],
\]

\[
= \frac{2\pi e^4 N Z}{m_e c^2 \beta^2} [1 - \ln(\tau Q_1) - \gamma]. \tag{3.34}
\]

When combining the integral expressions of low and high energy losses and including the
step length $s$ traveled, the expression of Eq. (3.28) becomes:

$$
\int_0^\infty w(Q)(1 - e^{-\tau Q})dQ = \tau \frac{2\pi e^4NZ}{m e^2 \beta^2} \left[1 - \gamma - \ln(sQ')\right],
$$

(3.35a)

$$
\int_0^\infty w(Q)(1 - e^{-\tau Q})dQ = \tau \xi \left[1 - \gamma - \ln(sQ')\right],
$$

(3.35b)

where

$$
\xi = \frac{2\pi e^4NZ}{m e^2 \beta^2} s.
$$

(3.36)

This expression does not account for the reduced energy loss of the primary electron because of the polarization from the background material, as discussed in Section 2.1.6. This polarization is incorporated by applying the density effect correction factor $\delta$ in an ad hoc manner:

$$
\int_0^\infty w(Q)(1 - e^{-\tau Q})dQ = \tau \xi \left[1 - \gamma - \delta - \ln(sQ')\right],
$$

(3.37)

Substituting Eq. (3.37) in Eq. (3.26) results in the Landau energy loss straggling distribution for a single material region [47]:

$$
f_L(s, \Delta) = \frac{1}{2\pi i} \int_{i\infty+\sigma}^{-i\infty+\sigma} \exp \left\{\tau \Delta - \tau \xi \left[1 - \gamma - \delta - \ln(sQ')\right]\right\} d\tau,
$$

(3.38)

When using the substitution $u = \tau \xi$, Eq. (3.38) becomes a universal function, which allows it to be applied to problems of various background material properties:

$$
f_L(s, \Delta) = \frac{1}{\xi} \phi(\lambda),
$$

(3.39a)

$$
\phi_L(\lambda) = \frac{1}{2\pi i} \int_{i\infty+\sigma}^{-i\infty+\sigma} e^{u \ln(u) + \lambda u} du,
$$

(3.39b)
Figure 3.1: Landau energy loss distribution as a function of the scaled energy loss parameter $\lambda$

where

$$
\lambda = \frac{\Delta - \xi \left[ \ln \left( \frac{\xi}{Q'} \right) + 1 - \gamma - \delta \right]}{\xi}.
$$

(3.40)

is a scaled parameter that contains the energy loss of the electron and is a function of background material properties and the kinetic energy of the electron. This solution must be numerically evaluated and is integrated over a line on the complex plane. This distribution has been tabulated for $\lambda \in [-4, 100]$ [10] and is provided in Figure 3.1.

Significant contribution to the integration value of Eq. (3.39a) occurs when the integration domain is near the real axis, which is around $u \approx 1$, and is used in the error analysis of Chechin and Ermilova (Section 3.3.3). Some notable shortcomings of this distribution are that it allows for negative energy loss $\Delta < 0$ and that the mean is infinite. A “fix-up” scheme for this distribution is discussed in Section 3.3.5.
3.3.2 Blunck & Leisegang

Based on experimental results obtained by White and Millington [106], Landau’s energy loss straggling distribution was shown to be inaccurate because of its narrow half-width. Blunck and Leisegang performed a correction on Landau’s energy loss straggling distribution to consider binding effects and improve the accuracy of the distribution. This correction begins by including the second-order Taylor series term for the small energy loss term, \(1 - e^{-\tau Q} \approx 1 - \tau Q + (\tau Q)^2/2:\)

\[
\begin{align*}
\int_0^\infty w(Q)(1 - e^{-\tau Q})dQ &= \int_0^{Q_1} w(Q) \left[ \tau Q - \frac{(\tau Q)^2}{2} \right] dQ + \int_{Q_1}^\infty w(Q)(1 - e^{-\tau Q})dQ, \\
&= s\tau \int_0^{Q_1} w(Q)QdQ - s\frac{\tau^2}{2} \int_0^{Q_1} w_1(Q)Q^2dQ + s \int_{Q_1}^\infty w(Q)(1 - e^{-\tau Q})dQ,
\end{align*}
\]

(3.41)

where \(w_1(Q)\) is the probability of energy loss from distant collisions and becomes less dominant at high kinetic energies (\(w_1(Q) \approx 1/Q^\nu, \nu \approx 4 - 5\)) [17]. To evaluate the second-order term, \(w_1\) is approximated using a Dirac delta function at point \(1.5I_s\), where \(I_s\) is the ionization potential of an electron in shell \(s\) and 1.5 is an estimate from the width of the resonance curves. The following expression is assumed such that the mean energy loss (first moment) \(\overline{Q}\) is recovered:

\[
\begin{align*}
\overline{Q}^2 &= \int_0^{Q_1} Q^2w_1(Q)dQ, \quad (3.42a) \\
w_1(Q) &= \sum_s \frac{\delta(Q - 1.5I_s)}{1.5I_s}, \quad (3.42b)
\end{align*}
\]
where according to the Bohr model [9], the mean energy loss over length traveled \( s \) is

\[
\bar{Q} = \sum_s Q_s = \frac{2\pi e^4 NZ}{m_e c^2 \beta^2} \sum_s \frac{R_s}{Z} \ln \left[ \frac{2mv^2}{I_s(1 - \beta^2)} \right].
\] (3.42c)

Here, \( R_s \) is the number of electrons of ionization potential \( I_s \). The second-order term evaluates to be

\[
\frac{s \tau^2}{2} \int_0^{Q_1} Q^2 w_1(Q) dQ = \frac{s \tau^2}{2} \bar{Q}^2,
\]

\[
= \frac{s \tau^2}{2} \int_0^{Q_1} Q^2 \left[ \sum_s Q_s \frac{\delta(Q - 1.5I_s)}{1.5I_s} \right] dQ
\]

\[
= \frac{s \tau^2}{2} \left[ 1.5 \sum_s I_s Q_s \right],
\]

\[
= \frac{s \tau^2}{2} \left\{ 1.5 \frac{2\pi e^4 NZ}{m_e c^2 \beta^2} \sum_s I_s \frac{R_s}{Z} \ln \left[ \frac{2mv^2}{I_s(1 - \beta^2)} \right] \right\},
\]

\[
= \frac{\tau^2}{2} \xi \left\{ 1.5 \sum_s I_s \frac{R_s}{Z} \ln \left[ \frac{2mv^2}{I_s(1 - \beta^2)} \right] \right\}. \quad (3.43)
\]

The Landau energy loss straggling distribution \( f_L(s, \Delta)ds \) is then convolved with a Gaussian with a mean of \( \bar{\tau} = 0 \) and variance of \( \sigma^2 = s\bar{Q}^2 \) to account for the dominant effect of \( \bar{Q}^2 \) on the broadening of the effective cross section distribution and to more accurately capture the Gaussian-like behavior of the experimental data identified by White and Millington [106]:

\[
g(x) = \frac{1}{\sqrt{2\pi \sigma^2}} \exp \left[ -\frac{(x - \bar{\tau})^2}{2\sigma^2} \right], \quad (3.44a)
\]

\[
f^*(s, \Delta) = \frac{1}{\sqrt{2\pi \sigma^2}} \int f_L(s, \Delta - x) \exp \left[ -\frac{x^2}{2\sigma^2} \right] dx. \quad (3.44b)
\]

Recall the universal expression of the Landau energy loss straggling distribution \( f_L(s, \Delta)ds = \phi(\lambda)d\lambda \) with the scaled energy-loss parameter \( \lambda \). Blunck and Leisegang numerically deter-
mined an approximate expression of \( \phi(\lambda) \) as the sum of Gauss functions:

\[
\phi(\lambda) = \sum_{\nu} c_{\nu} \gamma_{\nu} \frac{\exp \left[ -\left( \frac{\lambda - \lambda_{\nu}}{\gamma_{\nu}^2 + b^2} \right)^2 \right]}{\sqrt{\gamma_{\nu}^2 + b^2}},
\]

(3.45)

where, for one material region, the standard deviation is

\[
b_{BL} = \sqrt{\frac{2Q^2}{(2\pi e^4NZ)^2 s}} = \sqrt{\frac{2sQ^2}{\xi}} = \frac{\sqrt{2\sigma^2}}{\xi},
\]

(3.46)

and the constants \( c_{\nu}, \gamma_{\nu}, \) and \( \lambda_{\nu} \) were determined numerically and are provided in Table 3.2.

Blunck and Westphal later approximate Eq. (3.46) as a simpler expression [8] using the Thomas-Fermi atomic model [27, 93]:

\[
b_{BL} \approx b_{BW} = Z^{2/3} \sqrt{10 \text{ eV} \cdot \Delta},
\]

(3.47)

where \( \Delta \) is the mean energy loss over the length traveled \( s \).

3.3.3 Chechin & Ermilova

Chechin and Ermilova later derived an estimate for the relative error of the energy loss straggling distribution as a result of neglecting higher-order moments [17]. The authors derived this estimated relative error for Landau’s energy loss straggling distribution as well as Blunck and Leisegang’s accuracy improvement. They found that the second-order Taylor series term that was included in Blunck and Leisegang’s work resulted in modest improvements and conducted an error analysis that included the third-order Taylor series term for...
the small energy loss term, \( 1 - e^{-\tau Q} \approx 1 - \tau Q + (\tau Q)^2/2 - (\tau Q)^3/6 \):

\[
\int_0^{Q_1} w(Q)(1 - e^{-\tau Q})dQ = s \int_0^{Q_1} w(Q) \left[ \tau Q - \frac{(\tau Q)^2}{2} + \frac{(\tau Q)^3}{6} \right] dQ,
\]

\[
= s \tau \int_0^{Q_1} w(Q)dQ - \frac{s \tau^2}{2} \int_0^{Q_1} w_1(Q)Q^2dQ + \frac{s \tau^3}{6} \int_0^{Q_1} w_1(Q)Q^3dQ.
\]

(3.48)

Utilizing the empirical model proposed by Blunck and Leisegang in Eq. (3.42), the second-order expression yields Eq. (3.43). The third-order term evaluates to be

\[
\int_0^{Q_1} w_1(Q)Q^2dQ = \int_0^{Q_1} w_1(Q)Q^3dQ = \tau^2 \xi I \ln(a),
\]

(3.49a)

Using a weighted-average of the excitation potential to preserve the mean logarithmic excitation potential of matter, the second- and third-order terms simplify to

\[
\int_0^{Q_1} w_1(Q)Q^2dQ = \frac{\tau^2}{2} \xi I \ln(a),
\]

(3.50a)

\[
\int_0^{Q_1} w_1(Q)Q^3dQ = \frac{\tau^3}{6} \xi I^2 \ln(a),
\]

(3.50b)
where

\[ \ln(I) = \sum_s \frac{R_s}{Z} \ln(I_s), \]  
\[ \ln(a) = \beta^2 - \ln(Q') + \ln(I). \]  
\[ (3.51a) \]
\[ (3.51b) \]

The second-order term from Blunck and Leisegang’s work, Eq. (3.50a), can be used as an estimated correction to the Landau formula with the relationship \( \tau_L \approx \frac{1}{\xi} \). This relationship arises from the integration variable \( u = \tau \xi \) in Landau’s work, where \( u \approx 1 \) is the integration region of significant contribution to \( \phi_L(\lambda) \). The estimated second-order correction to the Landau distribution is of the order

\[ \epsilon_{BL} \approx \frac{\tau^2}{2} \xi I \ln(a), \]
\[ \approx \tau_L^2 \xi I \ln(a), \]
\[ = \frac{I \ln(a)}{\xi}, \]  
\[ (3.52) \]

where leading coefficients are dropped. If the second-order term from the Taylor-series expansion is included in the region of significance for integration \( u \approx 1 \), it takes the form \( u^2 = (\tau \xi)^2 + O(\tau^2) \approx 1^2 = 1 \), where \( O(\tau^2) \) is the second-order term from the Taylor-series expansion, Eq. (3.50a):

\[ u^2 = (\tau \xi)^2 + \frac{\tau^2}{2} \xi I \ln(a), \]
\[ 1 \approx \tau_B^2 \xi^2 + \tau_B^2 \xi I \ln(a), \]
\[ 1 = \tau_B^2 \left[ \xi^2 + \xi I \ln(a) \right], \]
\[ \Rightarrow \tau_B = \sqrt{\frac{1}{\xi I \ln(a) + \xi^2}}, \]  
\[ (3.53) \]
where, again, leading coefficients are dropped. Applying this relationship to the third-order term, Eq. (3.50b), yields the estimated third-order correction to the Landau distribution:

\[
\epsilon_{CE} \approx \tau_3^B \xi I^2 \ln(a),
\]

\[
= [\xi I \ln(a) + \xi^2]^{-3/2} [\xi I^2 \ln(a)],
\]

\[
= \left[ \frac{\xi}{I} \ln(a) \left( 1 + \frac{\xi}{I \ln(a)} \right) \right]^{-1/2}.
\]

(3.54)

### 3.3.4 Seltzer

Seltzer subsequently compared the Landau energy loss distribution with the Gaussian correction of Blunck and Leisegang to experimental data. In this work, Seltzer found that the ratio of the distributions’ full width half max (FWHM) of the computed results to the experimental results followed the error term Eq. (3.54) derived by Chechin and Ermilova and proposed a correction to the Blunck-Westphal variance [85]:

\[
\sigma = \frac{b_{BL}}{1 + 3 \epsilon_{CE}} = \frac{b_{BW}}{1 + 3 \epsilon_{CE}},
\]

(3.55)

to incorporate this error term and further improve the accuracy of the energy loss distribution.

### 3.3.5 Energy Loss Sampling

A well-known challenge with the Landau energy loss straggling distribution is that the mean of the distribution is infinite and therefore cannot preserve the mean energy loss of the particle. To preserve this mean energy loss \( \bar{\Delta} \), this work uses the traditional technique of truncating the distribution, which is currently used in standard condensed history methods. This technique truncates the distribution at \( \Delta < 0 \) such that energy gain is not permitted, and it truncates the tail of the distribution at a collisional energy loss \( \Delta_{\text{max}} \) such that
Eq. (3.56) holds true:

\[
\bar{\Delta} = \int_{s_n}^{s_{n+1}} \left( \frac{dE}{dx} \right)_{col} dx = \int_0^{\Delta_{\text{max}}} \Delta f(\Delta) d\Delta, \quad (3.56)
\]

where \( s = s_{n+1} - s_n \) is the step length.

To sample from this truncated energy loss straggling distribution, this distribution is first tabulated for discrete energy losses \( \Delta \in [0, \Delta_{\text{max}}] \). A random number \( \xi \in [0,1] \) is then sampled such that

\[
f(\Delta_i) < \xi < f(\Delta_{i+1}), \quad (3.57)
\]

where \( f(\Delta_i) \) is the value of the truncated energy loss straggling distribution at energy loss \( \Delta_i \). A piecewise-linear interpolation scheme is then used to compute the energy loss corresponding to \( \xi \):

\[
\Delta_\xi = \Delta_i + (\Delta_{i+1} - \Delta_i) \frac{\xi - f(\Delta_i)}{f(\Delta_{i+1}) - f(\Delta_i)}. \quad (3.58)
\]

### 3.4 Secondary Particle Production

As an electron moves through matter, it may interact with the background material and produce secondary electrons and photons, which are modeled as hard collisions and bremsstrahlung emissions in traditional condensed history algorithms. These respective events model electron inelastic collisions (described in Section 2.1.2) in which an electron ionizes an orbital electron, typically assumed to be a free electron, and bremsstrahlung photon emission (described in Section 2.1.3) in which an electron is decelerated by the electric field of a target nuclei and produces a photon as a result of energy conservation. Traditionally in a condensed history algorithm, secondary particle production via hard collisions and bremsstrahlung emission are handled in an analog manner at the end of each electron substep.
and are discussed in detail in this section.

### 3.4.1 Hard Collision Electrons

Hard collisions are when electrons experience a collision that results in a large change in energy and direction. These collisions do not occur as frequently as soft collisions, which are frequent and highly forward-peaked scatters that result in small changes in energy and direction. Hard collisions are sampled explicitly at the end of each substep \( s \), based on the mean free path of a hard collision in the background material. This mean free path is computed using the Møller [62] and Bhabha [6] cross sections, described in Eqs. (2.19b) and (2.22), respectively:

\[
\lambda_{hc} = \frac{1}{N\sigma_{in,i}},
\]

where \( N \) is the number density of the target. If a hard collision occurs, the direction of the secondary electron is determined using momentum conservation assuming a free target electron, and its outgoing kinetic energy is sampled using the energy transfer distributions described in Eqs. (2.19a) or (2.21), depending on the incident particle.

For a Class I condensed history algorithm, the energy and direction of the primary particle do not change after the event of a hard collision because these effects are already considered in the multiple-scattering theories for angular deflection and energy loss. For a Class II condensed history algorithm, both the energy and direction of the primary particle are affected by this process. Though this work focuses on Class I condensed history algorithms, both Class I and Class II condensed history algorithms are discussed in more detail in Sections 3.5.1 and 3.5.2.

The distance to a hard collision \( d_{hc} \) may be sampled using the probability density

\[
f(d_{hc}) = \frac{1}{\lambda_{hc}} \exp \left( -\frac{d_{hc}}{\lambda_{hc}} \right),
\]

where \( \lambda_{hc} = \frac{1}{N\sigma_{in,i}} \).
by inverting this expression to obtain

\[ dh_c = -\lambda_{hc} \ln(\xi), \]  

where \( \xi \in [0, 1] \) is a uniformly distributed random number and

\[ m_{hc} = -\ln (\xi) \]  

is the number of mean free paths. In this work, hard collision events are sampled by sampling the number of mean free paths, Eq. (3.62) and decrementing this value by the number of mean free paths \( s/\lambda_{hc} \) traveled by the electron after each substep \( s \).

### 3.4.2 Bremsstrahlung Photons

Energy loss due to the production of bremsstrahlung photons is important to consider especially for high energy electrons traversing high \( Z \) materials. Traditionally in a condensed history algorithm for a homogeneous background material, the production and location of bremsstrahlung photons are sampled according to a Poisson and uniform distribution, respectively, at the end of each substep. The mean number of photons emitted per unit path length is

\[ \frac{1}{\lambda_{br}} = N \int_{\epsilon_c}^{E} \frac{d\sigma_{br}}{dE'} dE', \]  

where \( N \) is the number density and \( d\sigma_{br}/dE \) is the single differential cross section in Eq. (2.28). The event of bremsstrahlung emission is sampled at the end of each electron substep from the probability

\[ P_{br} = \exp \left( -\frac{s}{\lambda_{br}} \right). \]
If bremsstrahlung emission occurs, its location is sampled uniformly within the substep traveled by the electron. The scattering angle and energy of the photon and incident electron are sampled from tabulated data, which are derived from the radiative stopping power, Eq. (2.34). The energy of the bremsstrahlung photon is then deducted from the electron energy.

Unlike the treatment of hard collisions in the Class I algorithm, the change in energy and direction of the primary electron must be adjusted after a bremsstrahlung photon emission. This is because radiative collisions are not considered in the multiple-scattering theories for angular deflection and energy loss and must be accounted for explicitly.

### 3.5 Condensed History Algorithms

There are two notable classes of a condensed history method: Class I and Class II [5]. Each relies on a path length, energy loss, angular deflection, and spatial deflection to adequately simulate a condensed electron track. The main difference between the two classes is that Class I uses developed multiple scattering theories to condense all possible electron interactions into some set step length, which is defined based on some mean energy loss, whereas Class II distinguishes soft collisions from hard collisions and defines the path length based on the next hard electron interaction. The main advantage of using the Class II condensed history method is that it is more accurate than the Class I condensed history method with a disadvantage being that it more complex. This work focuses on the Class I condensed history method.
3.5.1 Class I Algorithm

For a Class I condensed history algorithm, the path length is computed based on a mean energy loss. The relationship between energy and path length is

\[
E_{m-1} - E_m = - \int_{s_m^{-1}}^{s_m} \frac{dE}{ds} ds,
\]

(3.65)

where \(E_m\) is the energy of the electron at step \(m\), \(s_m\) is the path length at step \(m\), and \(-\frac{dE}{ds}\) is the total stopping power. The path length is commonly chosen such that the following condition is satisfied:

\[
\frac{E_m}{E_{m-1}} = k,
\]

(3.66)

where \(k = 2^{-1/8}\) is typically used because it results in a mean energy loss of 8.3% per step length and marginal changes in the mean angular deflection between steps [5]. As an electron streams, it experiences statistical fluctuations in energy loss for a given pathlength traveled because charged particles lose discrete amounts of energy as a result of ionization losses. The collisional stopping power is therefore used to sample the energy loss straggling quantity for a major step length from the Landau distribution, discussed in Section 3.3. This sampled energy loss is then divided by the number of substeps \(l\) taken for each major step to get the mean energy loss per substep \(
hoverline{\Delta}\). The length of each step length is also divided by the number of substeps to get the substep length \(s/l\). The electron’s direction of flight changes at the end of each substep, when an angular deflection is sampled from the Goudsmit-Saunderson distribution, discussed in Section 3.2. An electron history continues to stream until it escapes from the domain or until its kinetic energy drops belows a certain energy cutoff. In the event that the electron kinetic energy falls below this threshold, all of its energy is deposited. An energy cutoff of 1 keV is typically used because condensed history methods become an inadequate model in this energy regime, and single-scatter transport is required. Radiative stopping power and all catastrophic events are accounted for, and
the random walk of secondary photons and electrons produced during each history are then simulated. The Class I condensed history method can be implemented with variation in the algorithm and could follow the track described in Algorithm 1.

**Algorithm 1** Class I condensed history algorithm

1: Initialize electron
2: while $E > 1$ keV do
3:   Compute major step length $s$ using collisional stopping power $(\frac{dE}{dx})_{col}$
4:   Sample energy loss per major step $\Delta$ from Landau distribution $\phi(\lambda)$
5:   Compute substep length $\frac{\Delta}{m}$ and mean energy loss per sub step $\overline{\Delta} = \frac{\Delta}{m}$
6:   for each substep $m$ do
7:     Sample distance to boundary $d_b$
8:     Stream particle to $d = \min\{d_b, \frac{s}{m}\}$
9:     if $d == \frac{s}{m}$ then
10:        Deduct mean energy loss per sub step $\overline{\Delta}$ from current electron energy $E$
11:        Sample catastrophic events and store produced photons and electrons
12:        Sample angular deflection from Goudsmit-Saunderson distribution $F(\mu)$
13:        if $E < 1$ keV then
14:           Deposit electron energy $E$
15:           Break
16:        else
17:           Terminate electron
18:       Break
19:   Simulate random walk of produced photons and secondary electrons

### 3.5.2 Class II Algorithm

The Class II condensed history algorithm condenses the electron track based on catastrophic events, which result in large energy loss fractions, and it assumes a continuous energy loss rate between these interactions. This algorithm determines the path length of the electron from a pathlength distribution $P(s)$ that is a function of the collisional stopping power $(dE/dx)_{col}$ and the hard collision cross section $\Sigma_{in,i}$:

$$P(s)ds = e^{-Q(s)}dQ,$$  \hspace{1cm} (3.67)

$$Q(s) = \int_{E_{n+1}}^{E_n} \Sigma_{in,i} \left( \frac{ds}{dE} \right)_{col} dE.$$  \hspace{1cm} (3.68)
Here, $E_{n+1}$ is the kinetic energy of the electron prior to the $(n + 1)^{th}$ catastrophic event, which is determined from an exponential distribution based on $E_n$, the kinetic energy of the electron after the $n^{th}$ catastrophic event.

The algorithm begins by initializing an electron and sampling the step size of the electron using Eq. (3.67). The electron continues to stream with the continuous-slowing-down approximation using the step and substep scheme as described in Section 3.5.1, where the mean collisional energy loss is determined for a step length (energy loss straggling is not considered) and the angular deflection is sampled at the end of each substep. This continues until a catastrophic collision occurs and the energy loss fraction is sampled. A new step size is sampled based on the current state of the electron and this process repeats until the kinetic energy of the electron falls below the energy cutoff or until the electron leaks. An electron modeled with the Class II condensed history method could follow the track described in Algorithm 2.
\textbf{Algorithm 2} Class II condensed history algorithm

1: Initialize electron
2: \textbf{while} $E > 1$ keV \textbf{do}
3: \hspace{1em} Sample major step length $s$ using collisional stopping power \( \left( \frac{dE}{dx} \right)_{\text{col}} \)
4: \hspace{1em} Determine energy loss per major step $\Delta$ from collisional stopping power \( \left( \frac{dE}{dx} \right)_{\text{col}} \)
5: \hspace{1em} Compute substep length $\frac{s}{n}$ and mean energy loss per sub step $\overline{\Delta} = \frac{\Delta}{n}$
6: \hspace{1em} \textbf{for} each substep $m$ \textbf{do}
7: \hspace{2em} Sample distance to boundary $d_b$
8: \hspace{2em} Stream particle to $d = \min\{d_b, \frac{s}{n}\}$
9: \hspace{2em} \textbf{if} $d == \frac{s}{n}$ \textbf{then}
10: \hspace{3em} Deduct mean energy loss per sub step $\overline{\Delta}$ from current electron energy $E$
11: \hspace{3em} Sample angular deflection from Goudsmit-Saunderson distribution $F(\mu)$
12: \hspace{3em} Sample catastrophic collision $\text{flCollide}$
13: \hspace{3em} \textbf{if} $\text{flCollide} == \text{True}$ \textbf{then}
14: \hspace{4em} Sample energy loss $\Delta_{HC}$ and deduct from current electron energy $E$
15: \hspace{4em} Store secondary particle
16: \hspace{4em} \textbf{if} $E < 1$ keV \textbf{then}
17: \hspace{5em} Deposit electron energy $E$
18: \hspace{5em} Break
19: \hspace{4em} \textbf{if} $E < 1$ keV \textbf{then}
20: \hspace{5em} Deposit electron energy $E$
21: \hspace{5em} Break
22: \hspace{3em} \textbf{else}
23: \hspace{4em} Terminate electron
24: \hspace{4em} Break
25: \hspace{1em} Simulate random walk of secondary particles
CHAPTER 4

Condensed History Model for Stochastic Media

Current condensed history methods assume a uniform background material and do not account for material boundary crossings. This makes electron transport problems in stochastic media inaccessible to standard condensed history methods. This chapter proposes new derivations and methodologies to accurately account for the condensed history transport of electrons in binary, Markovian-mixed media. In this chapter, we conduct novel derivations of multi-scatter distributions that are generalized to multiple materials, describe how secondary particle production is evaluated in a random mixture, and propose a novel methodology to approximate the material-dependent energy deposition of electrons. We note that these derivations and methodologies reduce to the derivations and methodologies discussed in Chapter 3 for a uniform background material.

4.1 Binary Markovian Mixtures

This work focuses on electron transport in binary, Markovian mixtures, partly due to the prevalence of this material mixing type within the research topic of neutron transport methods in stochastic media. Markovian mixing statistics in the spatial domain also follow the same mathematics as homogeneous, continuous-time Markov chains in the time domain [77]. According to the Palm-Khinchin theorem, Markovian mixing statistics is a limiting case for other random processes under the assumption that many random material realizations are
considered during a simulation, which motivates the use of this model in this work.

4.1.1 Mathematical Model of Binary Markovian Mixtures

Markovian mixing is a renewal process, and a binary, Markovian-mixed realization can be characterized by exponentially distributed chord lengths $\Lambda_i$ of each material $i \in \{0, 1\}$. The probability of a point being material 0 and 1 can be computed as a function of its distance from another point, where the probability of the previous point being material 0, $q_0$, or 1, $q_1$, is known. The following set of first-order ODEs preserves the material probabilities along a pathlength by enforcing a balance between the rate at which a material transitions between 0 and 1 as a function of distance $s$:

$$\frac{d}{ds} P_0(s) - \frac{1}{\Lambda_0} P_0(s) + \frac{1}{\Lambda_1} P_1(s) = 0, \quad (4.1a)$$

$$\frac{d}{ds} P_1(s) + \frac{1}{\Lambda_0} P_0(s) - \frac{1}{\Lambda_1} P_1(s) = 0, \quad (4.1b)$$

where $P_0(s)$ and $P_1(s)$ are the probabilities of being in material 0 and 1, respectively, and the initial conditions are $P_0(0) = q_0$ and $P_1(0) = q_1 = 1 - q_0$. The solution to this system of equations is used during the condensed history algorithm for electron transport in binary, Markov media to preserve the material probabilities at each electron substep and is

$$P_0(s, q_0) = P_0 - (P_0 - q_0) e^{-\frac{s}{\Lambda_c}}, \quad (4.2a)$$

$$P_1(s, q_0) = P_1 + (P_0 - q_0) e^{-\frac{s}{\Lambda_c}}, \quad (4.2b)$$

where $s$ is the distance traveled and $P_0 = \Lambda_0 / (\Lambda_0 + \Lambda_1)$ and $P_1 = 1 - P_0$ are material volume fractions computed from material mean chord lengths $\Lambda_0$ and $\Lambda_1$. Here, $\Lambda_c$ is the correlation length of the binary mixture [73]:

$$\Lambda_c = \frac{\Lambda_0 \Lambda_1}{\Lambda_0 + \Lambda_1}, \quad (4.3)$$
which describes the coarseness of the material mixing and can be described as the effective chord length of the binary mixture. As $\Lambda_c \to 0$, the mixing approaches the limit of homogeneously mixed material properties at the atomic level, as assumed in the AM approximation, and the ergodic, asymptotic material probabilities are recovered from Eqs. (4.2):

$$P_i = \frac{\Lambda_i}{\Lambda_0 + \Lambda_1}. \quad (4.4)$$

This is also called the material volume fraction and is the probability of sampling material $i$ at any arbitrary random point within a binary mixture.

4.1.2 Generation Methods for Binary Markovian Realizations

A one-dimensional, binary, Markovian-mixed realization can be generated using one of two more common approaches. One is a “pseudo-interface” approach [71, 92], which relies on the correlation length of the mixture to define nodes within the domain. These nodes indicate where a material boundary may be and are called pseudo-interfaces because the material properties on each side of a node are not necessarily different. The mean number of pseudo-interfaces $I$ within length $s$ is

$$I = \frac{s}{\Lambda_c}. \quad (4.5)$$

Because the mean number of pseudo-interfaces is known, the frequency of $k$ pseudo-interfaces within a realization of length $s$ is determined using a Poisson distribution:

$$f(k, I) = e^{-I} \frac{I^k}{k!}. \quad (4.6)$$

Using a pseudo-interface approach to generate a one-dimensional, binary, Markovian realization, the $k$ pseudo-interfaces are randomly and uniformly distributed within a realization, and the material type in each cell defined by these pseudo-interfaces is sampled according
to the material volume fraction in Eq. (4.4).

Another approach successively samples exponentially distributed chord lengths of alternating material type until a desired length is achieved. The exponential chord length distribution is

\[ f(\lambda_i) = \frac{1}{\Lambda_i} \exp \left( -\frac{1}{\Lambda_i} \lambda_i \right), \]  

(4.7)

and the chord length may be sampled by inverting this distribution:

\[ \lambda_i = -\Lambda_i \ln(\xi), \]  

(4.8)

where \( \lambda_i \) is the sampled chord length of material \( i \) and \( \xi \in [0, 1] \) is a uniformly sampled random number. Figure 4.1 depicts this generation method in which exponentially distributed chord lengths of alternating material types 0 and 0 are successively sampled until a desired length \( s \) is reached for a single binary, Markovian-mixed material realization.

![Figure 4.1: Successive sampling of exponentially distributed chord lengths of alternating materials to generate a single material realization of length \( s \)](image-url)
4.1.3 Transit Length Distribution for Binary Markovian-Mixed Media

The exponentially distributed switching of material types along a path as described in Section 4.1.2 is analogous to another well-known random process called the telegraph process. In the telegraph process, a particle moves along a one-dimensional line with some speed in a forward or backward direction and switches directions at exponentially distributed times. This process of switching directions at exponentially distributed times in the telegraph process is analogous to the crossing from one material into another at exponentially distributed lengths when generating a material realization. Because of this correspondence, the probability density for the total length traveled in a material type, the transit length distribution, can be derived. In this work, this derived transit-length distribution is used to precompute ensemble-average distributions that account for all the possible material realizations an electron may travel through within a step or substep length while preserving the expectation. To the knowledge of the author, the connection to the telegraph process and the associated transit length distribution has not yet been applied in the context of transport in stochastic media and is a novel contribution of this work.

To derive the transit length distribution, let \( L_0 \) be a random variable that describes the total distance traveled in material 0 given the particle travels a total distance \( s \). Let \( L_1 = s - L_0 \) be a random variable that describes the total distance traveled in material 1 given the particle travels a total distance \( s \). The difference in the total distance traveled in material 0 and material 1 by a particle traveling a total distance \( s \) may then be described by the random variable

\[
X = L_0 - L_1 \\
= L_0 - (s - L_0) \\
= 2L_0 - s. \tag{4.9}
\]

We now begin with the following system of PDEs, which describes the switching of materials
at exponentially distributed distances \cite{75}, and initial conditions:

\[
\begin{align*}
\frac{\partial}{\partial s} p_m^0(x, s) + \frac{\partial}{\partial x} p_m^0(x, s) &= -\frac{1}{\Lambda_0} p_m^0(x, s) + \frac{1}{\Lambda_1} p_{m-1}^1(x, s), \quad m \geq 1, \\
\frac{\partial}{\partial s} p_m^1(x, s) - \frac{\partial}{\partial x} p_m^1(x, s) &= -\frac{1}{\Lambda_1} p_m^1(x, s) + \frac{1}{\Lambda_0} p_{m-1}^0(x, s), \quad m \geq 1,
\end{align*}
\]

Here, \( p_m^i(x, s) \) is the probability density of the difference in the total distance traveled in each material \( x = l_0 - l_1 = 2l_0 - s \) by the particle when starting in material \( i \in \{0, 1\} \) and experiencing \( m \) material changes within a total distance traveled \( s \), and \( \Lambda_i \) is the material mean chord length of material \( i \). In Eqs. (4.10), \( s \) corresponds to the total process time of a telegraph process, \( x \) corresponds to the net displacement of the particle in a telegraph process, and \( \Lambda_0 \) and \( \Lambda_1 \) correspond to mean time spent in the forward and backward direction in a telegraph process before switching directions.

For a particle that experiences \( m = 0 \) material switches within a length \( s \), the distribution \( p_0^0(x, s) \) is that of a uniform, absorption-only transport problem for the respective materials 0 and 1 and initial conditions:

\[
\begin{align*}
\frac{\partial p_0^0(x, s)}{\partial s} + \frac{\partial p_0^0(x, s)}{\partial x} &= -\frac{1}{\Lambda_0} p_0^0(x, s), \\
p_0^0(x, 0) &= \delta(x)
\end{align*}
\]

and

\[
\begin{align*}
\frac{\partial p_0^1(x, s)}{\partial s} + \frac{\partial p_0^1(x, s)}{\partial x} &= -\frac{1}{\Lambda_1} p_0^1(x, s), \\
p_0^1(x, 0) &= \delta(x)
\end{align*}
\]

We solve for the distribution \( p_0^0(x, s) \) for a particle traveling in material 0 using the method
of characteristics. We begin by solving the characteristic equations and initial conditions:

\[
\frac{dx}{dt} = 1, \quad (4.13a)
\]

\[
\frac{ds}{dt} = 1, \quad (4.13b)
\]

\[
\frac{dp_0^0(x, s)}{dt} = -\frac{1}{\Lambda_0} p_0^0(x, s), \quad (4.13c)
\]

and

\[
x(0) = \alpha, \quad (4.13d)
\]

\[
s(0) = 0, \quad (4.13e)
\]

\[
p_0^0(0, 0) = f(\alpha). \quad (4.13f)
\]

The solution for Eqs. (4.13a) can be obtained by separation of variables, integrating both sides, and applying initial conditions:

\[
\int dx = \int dt
\]

\[
x(t) = t + C
\]

\[
x(0) = C = \alpha \Rightarrow x = t + \alpha, \quad (4.14a)
\]

and

\[
\int ds = \int dt
\]

\[
s(t) = t + C
\]

\[
s(0) = C = 0 \Rightarrow s = t. \quad (4.14b)
\]
\[
\frac{dp_0^0(x, s)}{p_0^0(x, s)} = -\frac{1}{\Lambda_0} dt \\
\int \frac{dp_0^0(x, s)}{p_0^0(x, s)} = -\int \frac{1}{\Lambda_0} dt \\
\ln[p_0^0(x, s)] = -\frac{1}{\Lambda_0} t,
\]
\[
p_0^0(x, s) = k \exp \left( -\frac{1}{\Lambda_0} t \right) = k \exp \left( -\frac{1}{\Lambda_0} s \right) \\
p_0^0(x, 0) = k \exp \left[ -\frac{1}{\Lambda_0}(0) \right] \\
= k = \delta(x) \\
\Rightarrow p_0^0(x, s) = \delta(x - s) \exp \left( -\frac{1}{\Lambda_0} s \right). \quad (4.14c)
\]

Following the same analysis for a particle traveling in material 0 and experiencing \( m = 0 \) material changes in a uniform, absorption transport problem yields the following distributions:

\[
p_0^0(x, s) = \exp \left( -\frac{s}{\Lambda_0} \right) \delta(x - s), \quad (4.15a) \\
p_1^0(x, s) = \exp \left( -\frac{s}{\Lambda_1} \right) \delta(x + s). \quad (4.15b)
\]

To solve for the probability density \( p_{m}^i(x, s) \) of \( m \geq 1 \) material switches, first, a change of variables is used to eliminate the absorption term \(-p_{m}^i(x, s)/\Lambda_i\) in Eqs. (4.10):

\[
p_{m}^0(x, s) = \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_{m}^0(x, s), \quad (4.16) \\
p_{m}^1(x, s) = \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q_{m}^1(x, s), \quad (4.17) \\
\nu = \frac{1}{2} \left( \frac{1}{\Lambda_0} - \frac{1}{\Lambda_1} \right). \quad (4.18)
\]
For \( i = 0 \), applying the change of variables yields

\[
\frac{\partial}{\partial s} \left\{ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s) \right\} + \frac{\partial}{\partial x} \left\{ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s) \right\}
= -\frac{1}{\Lambda_0} \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s) + \frac{1}{\Lambda_1} \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q_1^{m-1}(x, s). \tag{4.19}
\]

Applying chain-rule results in

\[
\exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \frac{\partial}{\partial s} q_0^m(x, s) + q_0^m(x, s) \frac{\partial}{\partial s} \left\{ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \right\}
+ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \frac{\partial}{\partial x} q_0^m(x, s) + q_0^m(x, s) \frac{\partial}{\partial x} \left\{ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \right\}
= -\frac{1}{\Lambda_0} \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s) + \frac{1}{\Lambda_1} \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q_1^{m-1}(x, s), \tag{4.20}
\]

which reduces to

\[
\exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \frac{\partial}{\partial s} q_0^m(x, s) + \left( -\frac{1}{\Lambda_0} + \nu \right) \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s)
+ \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \frac{\partial}{\partial x} q_0^m(x, s) - \nu \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s)
= -\frac{1}{\Lambda_0} \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q_0^m(x, s) + \frac{1}{\Lambda_1} \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q_1^{m-1}(x, s). \tag{4.21}
\]

Rearranging terms gives

\[
\exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] \left[ \frac{\partial}{\partial s} q_0^m(x, s) + \frac{\partial}{\partial x} q_0^m(x, s) \right] = \frac{1}{\Lambda_1} \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q_1^{m-1}(x, s). \tag{4.22}
\]
Following the same steps for \( i = 1 \) and reducing yields the following system of PDEs:

\[
\frac{\partial}{\partial s} q^m_0(x, s) + \frac{\partial}{\partial x} q^m_0(x, s) = \frac{1}{\Lambda_1} q^{m-1}_1(x, s), \quad (4.23a)
\]
\[
\frac{\partial}{\partial s} q^m_1(x, s) - \frac{\partial}{\partial x} q^m_1(x, s) = \frac{1}{\Lambda_0} q^{m-1}_0(x, s). \quad (4.23b)
\]

Applying the change of variables to the initial conditions and the distributions for \( m = 0 \) material changes

\[
p^m_0(x, 0) = 0 = \exp \left[ -\left( \frac{1}{\Lambda_0} + \nu \right) (0) - \nu x \right] q^m_0(x, 0), \quad (4.24a)
\]
\[
p^m_1(x, 0) = 0 = \exp \left[ -\left( \frac{1}{\Lambda_1} - \nu \right) (0) - \nu x \right] q^m_1(x, 0), \quad (4.24b)
\]
\[
p^0(x, s) = \exp \left( -\frac{s}{\Lambda_0} \right) \delta(x - s) = \exp \left[ -\frac{s}{\Lambda_0} + \nu(s - x) \right] q^0_0(x, s), \quad (4.24c)
\]
\[
p^1(x, s) = \exp \left( -\frac{s}{\Lambda_1} \right) \delta(x + s) = \exp \left[ -\frac{s}{\Lambda_1} - \nu(x + s) \right] q^1_1(x, s), \quad (4.24d)
\]

we obtain

\[
q^m_0(x, 0) = 0, \quad m \geq 1, \quad (4.25a)
\]
\[
q^m_1(x, 0) = 0, \quad m \geq 1, \quad (4.25b)
\]
\[
q^0_0(x, s) = \exp[\nu(x - s)] \delta(x - s), \quad (4.25c)
\]
\[
q^0_1(x, s) = \exp[\nu(x + s)] \delta(x + s). \quad (4.25d)
\]

The method of characteristics is used to solve the system of PDEs in Eq. (4.23) for \( m \) material changes. For \( i = 0 \), a characteristic line originating at point \( x = A \) at \( s = 0 \) is derived from
the characteristic equation

\[
\frac{dx}{1} = \frac{ds}{1} \\
\int dx = \int ds \\
x = s + A \\
A = x - s.
\] (4.26)

Along this line, \(s'\) is a parameterization variable that moves along \(s\) such that

\[
x(s') = s' + A \\
= s' + s' + (x - s) \\
= x - (s - s').
\] (4.27)

To find the solution \(q_m^0(x, s)\) at \((x, s)\), we move along the characteristic line to the initial condition \(s = 0\) with respect to \(s'\). This is represented by the following expression using the chain-rule:

\[
\frac{d}{ds'} g_m^0(x(s'), s') = \frac{d}{ds'} g_m^0(x(s'), s') \frac{d}{ds'} s' + \frac{d}{ds'} x(s') \frac{d}{dx} g_m^0(x(s'), s') \\
= \frac{d}{ds'} g_m^0(x(s'), s') + \frac{d}{dx} g_m^0(x(s'), s').
\] (4.28)

Notice that the right-hand side of Eq. (4.28) is of the same form of the left-hand side of Eq.(4.23). Therefore, the derivative of \(g_m^0(x(s'), s')\) with respect to \(s'\) can be equated to
Applying the initial condition \( q_0^m(x,0) = 0 \) results in the general solution

\[
q_0^m(x,s) = \frac{1}{\Lambda_1} \int_0^s q_1^{m-1}(x-(s-s'),s')ds'.
\] (4.30a)

The same analysis can be applied to \( q_1^m(x(s'),s') \) to obtain

\[
q_1^m(x,s) = \frac{1}{\Lambda_0} \int_0^s q_0^{m-1}(x+s-s',s')ds'.
\] (4.30b)

The solution for \( m = 0 \) direction changes, Eqs. (4.25), can be used to find the general solution for \( m \) material changes. For \( m = 1 \), the solution \( q_1^1(x,s) \) is

\[
q_1^1(x,s) = \frac{1}{\Lambda_0} \int_0^s q_0^0(x-(s-s'),s')ds'
\]

\[
= \frac{1}{\Lambda_0} \int_0^s \exp \{ \nu [(x-(s-s')) + s'] \} \delta [(x-(s-s')) + s'] ds'
\]

\[
= \frac{1}{\Lambda_0} \int_0^s \exp \{ \nu (x-s + 2s') \} \delta [x-s + 2s'] ds'
\]

\[
= \frac{1}{2 \Lambda_0} H[(s-x)(x+s)].
\] (4.31)
where the indicator function $H(z)$ is the Heaviside function:

$$H(z) := \begin{cases} 
1, & z > 0, \\
0, & z \leq 0.
\end{cases} \quad (4.32)$$

For $m = 2$, the solution $q_2^0(x, s)$ is

$$q_2^0(x, s) = \frac{1}{\Lambda_1} \int_0^s q_1^1(x + (s - s'), s') ds'$$
$$= \frac{1}{\Lambda_1} \int_0^s \frac{1}{\Lambda_0} \frac{1}{2} \left( s' - (x + (s - s')) \right) \left( (x + (s - s')) + s' \right) ds'$$
$$= \frac{1}{2} \frac{1}{\Lambda_0 \Lambda_1} \int_0^s H\{ [-s - x + 2s'][x + s] \} ds'$$
$$= \frac{1}{2^2} \frac{1}{\Lambda_0 \Lambda_1} (s - x) H[(s - x)(x + s)]. \quad (4.33)$$

For $m = 3$, the solution $q_3^1(x, s)$ is

$$q_3^1(x, s) = \frac{1}{\Lambda_0} \int_0^s q_0^2(x - (s - s'), s') ds'$$
$$= \frac{1}{\Lambda_0} \int_0^s \frac{1}{\Lambda_0 \Lambda_1} \frac{1}{2^2} \left( s' - [x - (s - s')] \right) H\{ [s' - [x - (s - s')]](x - (s - s')) + s' \} ds'$$
$$= \frac{1}{2^3} \frac{1}{\Lambda_0 \Lambda_1} \int_0^s (s - x) H\{ [s - x][x - s + 2s'] \} ds'$$
$$= \frac{1}{2^3} \frac{1}{\Lambda_0 \Lambda_1} (s - x)(x + s) H[(s - x)(x + s)]. \quad (4.34)$$
For $m$ material changes, the solution generalizes to be

\[ q_{2m+1}^m(x, s) = \frac{1}{2^{2m+1}} \frac{1}{\Lambda_0^m \Lambda_1^{m+1}} \frac{(s-x)^m(x+s)^m}{(m!)^2} H[(s-x)(x+s)], \quad s \geq 0 \]  

(4.35)

\[ q_{2m+1}^m(x, s) = \frac{1}{2^{2m+1}} \frac{1}{\Lambda_0^m \Lambda_1^{m+1}} \frac{(s-x)^m(x+s)^m}{(m!)^2} H[(s-x)(x+s)], \quad s \geq 0 \]  

(4.36)

\[ q_{2m}^0(x, s) = \frac{1}{2^{2m}} \frac{1}{\Lambda_0^m \Lambda_1^{m}} \frac{(s-x)^m(x+s)^m}{m!(m-1)!} H[(s-x)(x+s)], \quad s \geq 1 \]  

(4.37)

\[ q_{2m}^1(x, s) = \frac{1}{2^{2m}} \frac{1}{\Lambda_0^m \Lambda_1^{m}} \frac{(s-x)^m(x+s)^m}{m!(m-1)!} H[(s-x)(x+s)], \quad s \geq 1 \]  

(4.38)

For an even number of switches $2m$, the particle will leave each material $m$ times, which is accounted for in the terms $\Lambda_0^m$ and $\Lambda_1^m$. For an odd number of switches $2m + 1$, the particle will leave the starting material $m + 1$ times, which is accounted for in the exponential of the material mean chord length of the starting material. To find the probability density for starting materials $i \in \{0, 1\}$ that accounts for all possible combinations of material switches, we take the sum of all solutions for $m$ material changes:

\[ p_0(x, s) = \exp \left[ -\frac{s}{\Lambda_0} + \nu(s-x) \right] q_0(x, s), \]  

(4.39a)

\[ p_1(x, s) = \exp \left[ -\frac{s}{\Lambda_1} - \nu(x+s) \right] q_1(x, s), \]  

(4.39b)

where

\[ q_0(x, s) = \sum_{m=0}^{\infty} q_{2m}^m(x, s) \]

\[ = q_0^0(x, s) + \sum_{n=0}^{\infty} q_{2n}^1(x, s) + \sum_{n=1}^{\infty} q_{2n}^0(x, s) \]

\[ = \exp[\nu(x-s)\delta(x-s) + H[(s-x)(x+s)] \times \]

\[ \left\{ \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \frac{(s-x)^n(x+s)^n}{2^{2n} \Lambda_0^n \Lambda_1^n} + \sum_{n=1}^{\infty} \frac{1}{n!(n-1)!} \frac{(s-x)^{n-1}(x+s)^{n}}{2^{2n} \Lambda_0^n \Lambda_1^n} \right\} \]
Applying Eqs. (4.40) to Eqs. (4.39) and rearranging terms, the probability densities reduce

\[ q_1(x, s) = \sum_{m=0}^{\infty} q_1^m(x, s) \]

\[ = q_1^0(x, s) + \sum_{n=0}^{\infty} q_1^{2n+1}(x, s) + \sum_{n=1}^{\infty} q_1^{2n}(x, s) \]

\[ = \exp[\nu(x + s)]\delta(x + s) + H[(s - x)(x + s)] \times \]

\[ \left\{ \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{n!^2} \frac{(s - x)^n(x + s)^n}{2^n \Lambda_0^2 \Lambda_1^2} + \sum_{n=1}^{\infty} \frac{1}{n!(n - 1)!^2} \frac{(s - x)^n(x + s)^{n-1}}{2^n \Lambda_0^2 \Lambda_1^{n-1}} \right\} \]

\[ = \exp[\nu(x + s)]\delta(x + s) + H[(s - x)(x + s)] \times \]

\[ \left\{ \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{n!^2} \frac{(s - x)^{1/2}(x + s)^{1/2}}{2^n \Lambda_0^2 \Lambda_1^{1/2}} \right\}^{2n} + \sum_{n=0}^{\infty} \frac{1}{n!(n + 1)!^2} \frac{(s - x)^{n+1}(x + s)^n}{2^{n+1} \Lambda_0^{n+1} \Lambda_1^{n+1}} \]

\[ = \exp[\nu(x + s)]\delta(x + s) + H[(s - x)(x + s)] \times \]

\[ \left[ \frac{1}{2} \frac{1}{\Lambda_0^2 \Lambda_1^2} \right] \sum_{n=0}^{\infty} \frac{1}{n!} \frac{(s - x)^n(x + s)^n}{2^n \Lambda_0^2 \Lambda_1^{n+2}} \right] + \sum_{n=0}^{\infty} \frac{1}{n!(n + 1)!^2} \frac{(s - x)^{n+1}(x + s)^n}{2^{n+1} \Lambda_0^{n+1} \Lambda_1^{n+1}} \]

\[ = \exp[\nu(x + s)]\delta(x + s) + H[(s - x)(x + s)] \times \]

\[ \left[ \frac{1}{2} \frac{1}{\Lambda_0^2 \Lambda_1^2} \right] \sum_{n=0}^{\infty} \frac{1}{n!} \frac{(s - x)^n(x + s)^n}{2^n \Lambda_0^2 \Lambda_1^{n+2}} \right] + \sum_{n=0}^{\infty} \frac{1}{n!(n + 1)!^2} \frac{(s - x)^{n+1}(x + s)^n}{2^{n+1} \Lambda_0^{n+1} \Lambda_1^{n+1}} \]

Here, \( I_0(z) \) and \( I_1(z) \) are modified Bessel functions of the first kind as described in Eq. (2.11b):

\[ J_n(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!(m + n)!} \left( \frac{x}{2} \right)^{2m+n} \]

Applying Eqs. (4.40) to Eqs. (4.39) and rearranging terms, the probability densities reduce
to the overall probability densities

\begin{align*}
p_0(x, s) &= \exp\left(-\frac{s}{\Lambda_0}\right) \delta(x - s) + \exp\left[-\frac{s}{\Lambda_0} + \nu(s - x)\right] H[(s - x)(x + s)] \times \left[ \frac{1}{2} \frac{1}{\Lambda_0} I_0 \left( \frac{(s - x)(x + s)}{\Lambda_0 \Lambda_1} \right) + \frac{1}{2\sqrt{\Lambda_0 \Lambda_1}} \frac{x + s}{s - x} I_1 \left( \frac{(s - x)(x + s)}{\Lambda_0 \Lambda_1} \right) \right], \\
p_1(x, s) &= \exp\left(-\frac{s}{\Lambda_1}\right) \delta(x + s) + \exp\left[-\frac{s}{\Lambda_1} - \nu(x + s)\right] H[(s - x)(x + s)] \times \left[ \frac{1}{2} \frac{1}{\Lambda_1} I_0 \left( \frac{(s - x)(x + s)}{\Lambda_0 \Lambda_1} \right) + \frac{1}{2\sqrt{\Lambda_0 \Lambda_1}} \frac{s - x}{x + s} I_1 \left( \frac{(s - x)(x + s)}{\Lambda_0 \Lambda_1} \right) \right],
\end{align*}

(4.41a)

(4.41b)

which describe the difference in total distance traveled in each material \(x\) when a particle traveling a distance \(s\) begins in materials 0 and 1, respectively, after all possible material switches.

Let \(f_i(l_0, s)\) describe the probability density of a particle traveling a total distance \(l_0\) in material 0 when traveling a total distance \(s\). Applying Eq. (4.9), we can obtain the relationship [75]

\begin{align*}
f_0(l_0, s) &= 2p_0(2l_0 - s, s), \quad (4.42a) \\
f_1(l_0, s) &= 2p_1(2l_0 - s, s). \quad (4.42b)
\end{align*}
For a particle beginning in material 0, we apply Eq. (4.41a) to Eq. (4.42a) and reduce:

\[
\begin{align*}
  f_0(l_0, s) &= 2 \left\{ \exp \left( -\frac{s}{\Lambda_0} \right) \delta[(2l_0 - s) - s] \\
  &\quad + \exp \left[ -\frac{s}{\Lambda_0} + \nu[s - (2l_0 - s)] \right] H\{4[s - (2l_0 - s)][(2l_0 - s) + s]\} \times \\
  &\quad \left[ \frac{1}{\Lambda_0} \frac{1}{2} I_0 \left( \sqrt{\frac{s - (2l_0 - s)}{s - (2l_0 - s)}} \right) \right. \\
  &\quad \left. + \frac{1}{2\Lambda_0} \sqrt{\frac{(2l_0 - s) + s}{s - (2l_0 - s)}} I_1 \left( \sqrt{\frac{s - (2l_0 - s)}{s - (2l_0 - s)}} \right) \right] \right\} \\
  &= 2 \left\{ \exp \left( -\frac{s}{\Lambda_0} \right) \delta[2(l_0 - s)] + \frac{1}{2} \exp \left[ -\frac{s}{\Lambda_0} + 2\nu(s - s_0) \right] H[4l_0(s - s_0)] \times \\
  &\quad \left[ \frac{1}{\Lambda_0} I_0 \left( \sqrt{\frac{4l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) + \sqrt{\frac{1}{\Lambda_0\Lambda_1}} \sqrt{\frac{2l_0}{2(s - s_0)}} I_1 \left( \sqrt{\frac{4l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) \right] \right\} \\
  &= 2 \left\{ \exp \left( -\frac{s}{\Lambda_0} \right) \delta(l_0 - s) + \frac{1}{2} \exp \left[ -\frac{s}{\Lambda_0} + 2 \left\{ \frac{1}{2} \left( \frac{1}{\Lambda_0} - \frac{1}{\Lambda_1} \right) \right\} (s - l_0) \right] \times \\
  &\quad H[l_0(l_0 - s)] \left[ \frac{1}{\Lambda_0} I_0 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) + \sqrt{\frac{1}{\Lambda_0\Lambda_1}} \sqrt{\frac{l_0}{s - l_0}} I_1 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) \right] \right\} \\
  &= \exp \left( -\frac{s}{\Lambda_0} \right) \delta(l_0 - s) + \exp \left[ -\frac{s}{\Lambda_0} + \frac{s - l_0}{\Lambda_0} - \frac{s - s_0}{\Lambda_1} \right] H[l_0(l_0 - s)] \times \\
  &\quad \left[ \frac{1}{\Lambda_0} I_0 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) + \sqrt{\frac{1}{\Lambda_0\Lambda_1}} \sqrt{\frac{l_0}{s - l_0}} I_1 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0\Lambda_1}} \right) \right].
\end{align*}
\]

Applying the same analysis when starting in material 1 and reducing results in the final form of the probability densities of the total distance traveled in material 0 when beginning
in material indexed by 0 and 1, respectively [75]

\[
f_0(l_0, s) = \exp \left( -\frac{s}{\Lambda_0} \right) \delta(l_0 - s) + \exp \left( -\frac{l_0}{\Lambda_0} - \frac{s - l_0}{\Lambda_1} \right) H[l_0(l_0 - s)] \times \\
\left[ \frac{1}{\Lambda_0} I_0 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0 \Lambda_1}} \right) + \sqrt{\frac{1}{\Lambda_0 \Lambda_1}} \sqrt{\frac{l_0}{s - l_0}} I_1 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0 \Lambda_1}} \right) \right],
\]

(4.44a)

\[
f_1(l_0, s) = \exp \left( -\frac{s}{\Lambda_1} \right) \delta(l_0) + \exp \left( -\frac{l_0}{\Lambda_0} - \frac{s - l_0}{\Lambda_1} \right) H[l_0(l_0 - s)] \times \\
\left[ \frac{1}{\Lambda_1} I_0 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0 \Lambda_1}} \right) + \sqrt{\frac{1}{\Lambda_0 \Lambda_1}} \sqrt{\frac{s - l_0}{l_0}} I_1 \left( 2 \sqrt{\frac{l_0(s - l_0)}{\Lambda_0 \Lambda_1}} \right) \right].
\]

(4.44b)

For each expression in Eqs. (4.44), the first term containing the Dirac delta function accounts for a domain of a single material. The second term represents an infinite sum of all possible material realizations.

This transit-length distribution is used in this work to (i) homogenize the material in a manner that incorporates the underlying randomness of the background material and (ii) generate the multiple-scattering distributions. While this transit-length distribution accounts for all possible material realizations that a particle may travel through, it does not retain the order in which the particle passes through each material region. Because of this, this distribution does not retain the material-dependent energy loss of the particle as it travels through each material region along a given path length.

4.1.3.1 Atomic Mix Limit of the Transit Length Distribution for Binary Markovian-Mixed Media

Here, we perform an asymptotic analysis to demonstrate that the transit length distributions presented in Eqs. (4.44) preserve the Atomic Mix limit. This is also shown numerically in Chapter 5. We begin by formulating the transit length distribution \( f_0(l_0, s) \) as an equiv-
alent expression:

\[ f_0(l_0, s)dl_0 = \exp\left(-\frac{s}{\Lambda_0}\right)\delta(l_0 - s) + \exp\left(-\frac{l_0}{\Lambda_0} - \frac{s - l_0}{\Lambda_1}\right)H[l_0(l_0 - s)] \times \]

\[ \left[ \frac{1}{\Lambda_0} I_0(z) + \frac{1}{\Lambda_0\Lambda_1} \sqrt{\frac{l_0}{s - l_0}} I_1(z) \right] dl_0, \]  

(4.45a)

where

\[ z = 2\sqrt{\frac{l_0(s - l_0)}{\Lambda_0\Lambda_1}}. \]  

(4.45b)

We parameterize \(1/\Lambda_1\) in terms of \(1/\Lambda_0\):

\[ \frac{1}{\Lambda_1} = k \frac{1}{\Lambda_0}, \quad k > 0. \]  

(4.46)

We can now express the transit length distribution \(f_0(l_0, s)\) as

\[ f_0(l_0, s)dl_0 = \exp\left(-\frac{s}{\Lambda_0}\right)\delta(l_0 - s) + \exp\left(-\frac{l_0}{\Lambda_0} - \frac{k(s - l_0)}{\Lambda_0}\right)H[l_0(l_0 - s)] \times \]

\[ \left[ \frac{1}{\Lambda_0} I_0(z) + \frac{1}{\Lambda_0} \sqrt{\frac{kl_0}{s - l_0}} I_1(z) \right] dl_0, \]  

(4.47a)

\[ = \exp\left(-\frac{s}{\Lambda_0}\right)\delta(l_0 - s) + \frac{1}{\Lambda_0} \exp\left[-\frac{l_0 + k(s - l_0)}{\Lambda_0}\right]H[l_0(l_0 - s)] \times \]

\[ \left[ I_0(z) + \sqrt{\frac{kl_0}{s - l_0}} I_1(z) \right] dl_0, \]  

(4.47b)

and the argument of the Modified Bessel functions \(z\) as

\[ z = 2\sqrt{\frac{kl_0(s - l_0)}{\Lambda_0}}. \]  

(4.47c)
In the AM limit, \( \Lambda_0, \Lambda_1 \ll s \). This implies that \( 1/\Lambda_0 \to \infty \). Therefore, \( z \to \infty \). These asymptotic limits result in the following relations:

\[
\exp \left( -\frac{s}{\Lambda_0} \right) \to 0, \quad (4.48a)
\]

\[
I_{\nu}(z) \sim \frac{\exp(z)}{\sqrt{2\pi z}}. \quad (4.48b)
\]

Inserting Eqs. (4.48) and Eq. (4.47c) into Eq. (4.65) and rearranging terms gives

\[
f_0(l_0, s)dl_0 = \frac{1}{\alpha} \delta(l_0 - s) + \frac{1}{\alpha \Lambda_0} \exp \left[ -\frac{l_0 + k(s - l_0)}{\Lambda_0} \right] H[l_0(l_0 - s)] \times \frac{\exp(z)}{\sqrt{2\pi z}} \frac{\exp(z)}{\sqrt{2\pi z}} \frac{\exp(z)}{\sqrt{2\pi z}} dl_0,
\]

\[
\begin{align*}
= \frac{1}{\alpha} \frac{1}{\Lambda_0} \exp \left[ -\frac{l_0 + k(s - l_0)}{\Lambda_0} \right] H[l_0(l_0 - s)] \times \exp(z) \left( 1 + \sqrt{\frac{kl_0}{s - l_0}} \right) dl_0, \\
= \frac{1}{\alpha} \frac{1}{\Lambda_0 \sqrt{2\pi z}} \exp \left[ -\frac{l_0 + k(s - l_0)}{\Lambda_0} \right] H[l_0(l_0 - s)] \times \exp(z) \left( 1 + \sqrt{\frac{kl_0}{s - l_0}} \right) dl_0, \\
= \frac{1}{\alpha} \frac{1}{\Lambda_0 \sqrt{2\pi} \frac{2\sqrt{kl_0(s - l_0)}}{\Lambda_0}} \exp \left[ -\frac{2\sqrt{kl_0(s - l_0)}}{\Lambda_0} - \frac{l_0 + k(s - l_0)}{\Lambda_0} \right] \\
\times H[l_0(l_0 - s)] \left( 1 + \sqrt{\frac{kl_0}{s - l_0}} \right) dl_0, \\
= \frac{1}{\alpha} \frac{1}{2 \sqrt{\pi \Lambda_0 \sqrt{kl_0(s - l_0)}}} \exp \left[ -\frac{1}{\Lambda_0} \left( \sqrt{l_0} - \sqrt{k(s - l_0)} \right)^2 \right] H[l_0(l_0 - s)] \times \\
\left( \frac{\sqrt{s - l_0} + \sqrt{kl_0}}{\sqrt{s - l_0}} \right) dl_0, \quad (4.49)
\end{align*}
\]

where \( \alpha \) is a normalization factor, which must be introduced because normalization is not retained when applying Eq. (4.48b) to Eq. (4.65). Next, we reformulate Eq. (4.65) using the
substitution

\[ u = \sqrt{l_0} - \sqrt{k(s - l_0)}, \quad (4.50a) \]
\[ du = \frac{\sqrt{kl_0} + \sqrt{s - l_0}}{2\sqrt{l_0(s - l_0)}} dl_0 \]
\[ \Rightarrow dl_0 = \frac{2\sqrt{l_0(s - l_0)}}{\sqrt{kl_0} + \sqrt{s - l_0}} du, \quad (4.50b) \]

to get

\[ f_0(u, s) du = \frac{1}{\alpha} \sqrt{\frac{l_0}{\pi \Lambda_0 \sqrt{kl_0(s - l_0)}}} \exp \left( -\frac{u^2}{\Lambda_0} \right) H[l_0(l_0 - s)] du. \quad (4.51) \]

We use the substitution

\[ \frac{1}{\Lambda_0} = \frac{1}{\sigma^2}, \quad (4.52) \]

to get

\[ f_0(u, s) du = \frac{1}{\alpha} \sqrt{\frac{l_0}{\pi \sqrt{kl_0(s - l_0)}} \sqrt{\pi |\sigma|^2}} \exp \left( -\frac{u^2}{\sigma^2} \right) H[l_0(l_0 - s)] du. \quad (4.53) \]

In the limit as \(1/\Lambda_0 \to \infty\), we have \(\sigma \to 0\). Therefore, we then apply a definition of the Dirac delta function:

\[ \delta(z) = \lim_{\sigma \to 0} \frac{1}{\sqrt{\pi |\sigma|}} \exp \left( \frac{z^2}{\sigma^2} \right), \quad (4.54) \]

and the asymptotic form of Eq. (4.59) can be written:

\[ f_0(u, s) du = \frac{1}{\alpha} \sqrt{\frac{l_0}{\sqrt{kl_0(s - l_0)}}} \delta(u) H[l_0(l_0 - s)] du. \quad (4.55) \]
From Eq. (4.50a), we solve for $l_0$ as a function of $u$ and obtain

$$l_0 = \left[ \frac{u + \sqrt{(k+1)ks - ku^2}}{k+1} \right]^2. \quad (4.56)$$

For the asymptotic transit length distribution, we are interested in $l_0$ at $u = 0$ since the argument of the Dirac delta function is at $u = 0$, which is

$$l_0(u = 0) = \frac{ks}{k+1}. \quad (4.57)$$

Applying $l_0(u = 0)$ to the square root term in Eq. (4.55) yields

$$\sqrt{\frac{l_0(u = 0)}{\sqrt{k}l_0(u = 0)(s - l_0(u = 0))}} = \sqrt{\frac{ks}{k+1}(s - \frac{ks}{k+1})} = \left( \frac{ks}{k+1} \right)^{1/2} \left( k \left( \frac{ks}{k+1} \right) \left( s - \frac{ks}{k+1} \right) \right)^{-1/4}$$

$$= \left( \frac{ks}{k+1} \right)^{1/2} \left( k \left( \frac{ks}{k+1} \right) \left( \frac{ks + s - ks}{k+1} \right) \right)^{-1/4}$$

$$= \left( \frac{ks}{k+1} \right)^{1/2} \left( \left( \frac{ks}{k+1} \right) \left( \frac{ks}{k+1} \right) \right)^{-1/4} = 1, \quad (4.58)$$

and because the asymptotic distribution is zero everywhere except at $u = 0$, Eq. (4.55) can be written as

$$f_0(u)du = \delta(u)du, \quad (4.59)$$

which is a normalized distribution, and therefore, the normalization factor $\alpha$ may be eliminated. This result implies that in the AM limit, where $\Lambda_0, \Lambda_1 \ll s$, the transit length distribution converges to a Dirac delta function. Multiplying a quantity by Eq. (4.59) and integrating leads to quantities being evaluated at $u = 0$, and evaluating at $u = 0$ results in
quantities at the AM limiting transit length value

\[ l_0 = \frac{\Lambda_0 / \Lambda_1}{\Lambda_0 / \Lambda_1 + 1} s = \left( \frac{\Lambda_0}{\Lambda_0 + \Lambda_1} \right) s, \] (4.60)

where the term in parentheses is the material volume fraction, described in Eq. (4.4), of material 0, which is the AM limit.

A similar asymptotic analysis may be conducted using the transit length distribution \( f_1(l_0, s) \) when beginning in material 1, which also results in the material volume fraction of material 0. This analysis is shown here to illustrate differences compared to the asymptotic analysis conducted on \( f_0(l_0, s) \). We begin with

\[
f_1(l_0, s)dl_0 = \exp\left(-\frac{s}{\Lambda_1}\right) \delta(l_0) + \exp\left(-\frac{l_0}{\Lambda_0} - \frac{s - l_0}{\Lambda_1}\right) H[l_0(l_0 - s)] \times \left[ \frac{1}{\Lambda_1} I_0(z) + \sqrt{\frac{1}{\Lambda_0 \Lambda_1}} \sqrt{\frac{s - l_0}{l_0}} I_1(z) \right] dl_0,
\]

(4.61)

where \( z \) is described in Eq. (4.45b). Using the same parameterize described in Eq. (4.46), we express \( 1/\Lambda_0 \) in terms of \( 1/\Lambda_1 \):

\[
\frac{1}{\Lambda_0} = \frac{1}{k} \frac{1}{\Lambda_1}, \quad k > 0.
\]

(4.62)

We can now express the transit length distribution \( f_1(l_0, s) \) as

\[
f_1(l_0, s)dl_0 = \exp\left(-\frac{s}{\Lambda_1}\right) \delta(l_0) + \frac{1}{\Lambda_1} \exp\left[-\frac{l_0 + k(s - l_0)}{k \Lambda_1}\right] H[l_0(l_0 - s)] \times \left[ I_0(z) + \sqrt{\frac{s - l_0}{kl_0}} I_1(z) \right] dl_0,
\]

(4.63a)
and the argument of the Modified Bessel functions \( z \) as

\[
z = \frac{2}{\Lambda_1} \sqrt{\frac{l_0(s - l_0)}{k}}.
\] (4.63b)

In the AM limit, \( \Lambda_0, \Lambda_1 \ll s \). This implies that \( 1/\Lambda_1 \to \infty \). Therefore, \( z \to \infty \). These asymptotic limits, again, result in the following relations:

\[
\exp \left( -\frac{s}{\Lambda_1} \right) \to 0,
\] (4.64a)

\[
I_\nu (z) \sim \frac{\exp(z)}{\sqrt{2\pi z}}.
\] (4.64b)

Inserting Eqs. (4.64) and Eq. (4.63b) into Eq. (4.63a) and rearranging terms gives

\[
f_1(l_0, s)dl_0 = \frac{1}{\alpha} \frac{1}{\sqrt{\pi \Lambda_1 \sqrt{\frac{l_0(s - l_0)}{k}}}} \exp \left[ -\frac{1}{\Lambda_1} \left( \sqrt{\frac{l_0}{k}} - \sqrt{\frac{s - l_0}{k}} \right)^2 \right] H[l_0(l_0 - s)] \times
\]

\[
\left( \frac{\sqrt{s - l_0} + \sqrt{k l_0}}{\sqrt{k l_0}} \right) dl_0,
\] (4.65)

where \( \alpha \) is a normalization factor. Next, we reformulate Eq. (4.63a) using the substitution

\[
u = \sqrt{\frac{l_0}{k}} - \sqrt{s - l_0},
\] (4.66a)

\[
\frac{dv}{2} = \frac{\sqrt{k l_0} + \sqrt{s - l_0}}{2 \sqrt{k l_0(s - l_0)}} dl_0
\]

\[
\Rightarrow dl_0 = \frac{2 \sqrt{k l_0(s - l_0)}}{\sqrt{k l_0 + \sqrt{s - l_0}}} dv,
\] (4.66b)

to get

\[
f_1(u, s)du = \frac{1}{\alpha} \sqrt{\frac{s - l_0}{\pi \Lambda_1 \sqrt{\frac{l_0(s - l_0)}{k}}}} \exp \left( -\frac{u^2}{\Lambda_0} \right) H[l_0(l_0 - s)] du.
\] (4.67)
We then use the substitution \( \Lambda_1 = \sigma^2 \) to get

\[
f_1(u, s)du = \frac{1}{\alpha} \sqrt{\frac{s - l_0}{\frac{1}{k} l_0(s - l_0)}} \frac{1}{\sqrt{\pi |\sigma^2|}} \exp \left( -\frac{u^2}{\sigma^2} \right) H[l_0(l_0 - s)]du.
\]  
(4.68)

In the limit as \( 1/\Lambda_1 \to \infty \), we have \( \sigma \to 0 \). Therefore, we apply a definition of the Dirac delta function described in Eq. (4.54) to get the asymptotic form of Eq. (4.59):

\[
f_1(u, s)du = \frac{1}{\alpha} \sqrt{\frac{s - l_0}{\frac{1}{k} l_0(s - l_0)}} \delta(u)H[l_0(l_0 - s)]du.
\]  
(4.69)

From Eq. (4.66a), we solve for \( l_0 \) as a function of \( u \) and obtain

\[
l_0 = k \left[ u + \sqrt{(k + 1)ks - ku^2} \right]^2.
\]  
(4.70)

For the asymptotic transit length distribution, we are interested in \( l_0 \) at \( u = 0 \) since the argument of the Dirac delta function is at \( u = 0 \), which is

\[
l_0(u = 0) = \frac{ks}{k + 1}.
\]  
(4.71)

Applying \( l_0(u = 0) \) to the square root term in Eq. (4.69) yields

\[
\sqrt{\frac{s - l_0(u = 0)}{\frac{1}{k} l_0(u = 0)(s - l_0(u = 0))}} = 1,
\]  
(4.72)

and because the asymptotic distribution is zero everywhere except at \( u = 0 \), Eq. (4.69) can be written as

\[
f_1(u)du = \delta(u)du.
\]  
(4.73)

This result implies that in the AM limit, the transit length distribution converges to a Dirac
delta function leading to quantities being evaluated at $u = 0$ or a transit length of

$$l_0 = \left( \frac{\Lambda_0}{\Lambda_0/\Lambda_1 + 1} \right)^s,$$

$$= \left( \frac{\Lambda_0}{\Lambda_0 + \Lambda_1} \right)^s,$$

(4.74)

where, again, the term in parenthesis is the material volume fraction of material 0 as described in Eq. (4.4) and is the AM limit.

## 4.2 Angular Deflection in Binary Markovian-Mixed Media

### 4.2.1 Goudsmit & Saunderson

Goudsmit-Saunderson established the following multiple-scattering angular deflection distribution by assuming a homogeneous material throughout the entire substep length $s$ traveled:

$$F(s, E) = \sum_{l=0}^{\infty} \left( l + \frac{1}{2} \right) \exp\left[ -sG_l(E) \right] P_l(\mu),$$

(4.75a)

$$G_l(E) = 2\pi N \int_{-1}^{1} \frac{d\sigma}{d\Omega}(\mu', E)[1 - P_l(\mu')] d\mu'.$$

(4.75b)

In a Markovian mixture, the domain consists of random layers or zones of different materials with chord lengths that follow an exponential distribution. Following the derivation of Goudsmit and Saunderson, we derive a generalized distribution for the Legendre coefficients $G_l(E)$ of angular deflection coefficients representing the ensemble average of the transit lengths [99].

To begin, let $\mu_0$ and $\mu_1$ be the scattering cosines of two successive independent scatters in stochastic zones with materials 0 and 1 respectively, and $\gamma_0$ and $\gamma_1$ be the corresponding azimuthal angles. If $\mu$ is the cosine of the angle between the resulting direction vectors, then
the addition theorem of spherical harmonics gives

\[
P_\ell(\mu) = P_\ell(\mu_0)P_\ell(\mu_1) + 2 \sum_{m=1}^{\ell} \frac{(\ell - m)!}{(\ell + m)!} P^m_\ell(\mu_0)P^m_\ell(\mu_1) \cos[m(\gamma_0 - \gamma_1)].
\] (4.76)

The expectation of this can then be taken. Because the scattering process is azimuthally symmetric, the expectation of the second term is zero. Additionally, the angles between subsequent scatters are independent. Therefore,

\[
E[P_\ell(\mu)] = E[P_\ell(\mu_0)P_\ell(\mu_1)] \\
= E[P_\ell(\mu_0)]E[P_\ell(\mu_1)].
\] (4.77)

The addition theorem of spherical harmonics can be taken repeatedly to get the expectation of a large number of collisions since scatters are independent. Let \( k_0 \) and \( k_1 \) be the number of collisions in regions 0 and 1 respectively. The expectation of the Legendre polynomial for this case is

\[
E[P_\ell(\mu)] = E[P_\ell(\mu_0)]^{k_0}E[P_\ell(\mu_1)]^{k_1}.
\] (4.78)

To get the Legendre expansion coefficient for the mixture, it is necessary to average over all possible values of \( k_0 \) and \( k_1 \). Let \( W(k_0, k_1) \) be the probability that \( k_0 \) and \( k_1 \) scatters occur in the respective region. The expansion coefficient can be found by taking the expectation over all possible collision orders:

\[
G_\ell = \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} W(k_0, k_1)E[P_\ell(\mu_0)]^{k_0}E[P_\ell(\mu_1)]^{k_1}.
\] (4.79)
We can then write $W(k_0, k_1)$ as a marginal distribution of the random transit length $l_0$ in region 0, where the transit length in region 1 is parametrically determined by

$$l_0 + l_1 = s$$  \hspace{1cm} (4.80)

for fixed substep length $s$. This is

$$W(k_0, k_1) = \int_0^s W(k_0, k_1|l_0)f(l_0, s)dl_0, \hspace{1cm} (4.81)$$

where $f(l_0, s)$ is given by Eq. (4.44a) and is the transit-length probability density function for region 0, i.e., the probability per unit length that the electron travels a distance $l_0$ in region 0 within a substep of length $s$. In the condensed history method, the cross sections are assumed to be constant during each substep. Because the mean number of scatters in each material is known, the number of scatters in either zone can be modeled as a Poisson process, and the conditional distribution may be written as

$$W(k_0, k_1|l_0) = \left[ (\Sigma_0 l_0)^{k_0} \frac{e^{-\Sigma_0 l_0}}{k_0!} \right] \left[ (\Sigma_1 L_1)^{k_1} \frac{e^{-\Sigma_1 L_1}}{k_1!} \right]. \hspace{1cm} (4.82)$$
Inserting this into Eq. (4.79), evaluating the expression using the exponential power series expansion $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$, and using the relation $\Sigma_n = N\sigma_n$ for material $n$ gives

$$G_{\ell} = \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} \left[ \int_0^s W(k_0, k_1|l_0) f(l_0, s) dl_0 \right] E[P_{\ell}(\mu_0)]^{k_0} E[P_{\ell}(\mu_1)]^{k_1}$$

$$= \int_0^s f(l_0, s) \left[ \sum_{k_0=0}^{\infty} \left( \frac{\Sigma_0 l_0}{k_0!} e^{-\Sigma_0 l_0} E[P_{\ell}(\mu_0)]^{k_0} \right) \right] \left[ \sum_{k_1=0}^{\infty} \left( \frac{\Sigma_1 l_1}{k_1!} e^{-\Sigma_1 l_1} E[P_{\ell}(\mu_1)]^{k_1} \right) \right] dl_0$$

$$= \int_0^s f(l_0, s) e^{-\Sigma_0 l_0} \sum_{k_0=0}^{\infty} \left( \frac{\Sigma_0 l_0 E[P_{\ell}(\mu_0)]}{k_0!} \right) e^{-\Sigma_1 l_1} \sum_{k_1=0}^{\infty} \left( \frac{\Sigma_1 l_1 E[P_{\ell}(\mu_1)]}{k_1!} \right) dl_0$$

$$= \int_0^s f(l_0, s) \exp \left\{ -\Sigma_0 l_0 \right\} \exp \left\{ \Sigma_0 l_0 E[P_{\ell}(\mu_0)] \right\} \exp \left\{ -\Sigma_1 l_1 \right\} \exp \left\{ \{ \Sigma_1 l_1 E[P_{\ell}(\mu_1)] \} \right\} dl_0$$

$$= \int_0^s f(l_0, s) \exp \left\{ -\Sigma_0 l_0 \left[ 1 - E[P_{\ell}(\mu_0)] \right] \right\} \exp \left\{ -\Sigma_1 l_1 \left[ 1 - E[P_{\ell}(\mu_1)] \right] \right\} dl_0$$

$$= \int_0^s f(l_0, s) \exp \left\{ -\sum_{n=0}^{\infty} N_n \sigma_n l_n \left[ 1 - E[P_{\ell}(\mu_n)] \right] \right\} dl_0. \quad (4.83)$$

Using the relationship between the expectation of the Legendre polynomial and the DCS Legendre moment described in Eqs. (3.12) yields the Legendre moments of the multi-scatter angular deflection distribution for a binary Markovian-mixed realization:

$$F(s, \mu) = \sum_{l=0}^{\infty} \left( l + \frac{1}{2} \right) G_{\ell}(s) P_{\ell}(\mu), \quad (4.84a)$$

$$G_{\ell}(s) = \int_0^s f(l_0, s) \exp \left\{ -2\pi \sum_{n=0}^{\infty} N_n \sigma_n \int_{-1}^{1} \frac{d\sigma_n}{d\Omega}(\mu') [1 - P_{\ell}(\mu')] d\mu' \right\} dl_0. \quad (4.84b)$$
4.3 Energy Loss Straggling in Binary Markovian-Mixed Media

4.3.1 Landau

Landau derived a solution to the energy loss function for an electron traversing a single material in the following form:

$$f_L(s, \Delta) = \frac{1}{2\pi i} \int_{i\infty + \sigma}^{i\infty - \sigma} \exp \{\tau \Delta - \tau \xi [1 - \gamma - \delta - \ln(sQ')]\} d\tau.$$ (4.85)

Here, we derive a generalized energy loss straggling distribution for an electron traversing multiple materials [100]. We begin with the governing conservation equation described in Eq. (3.19) and assume a space-dependent probability of an energy loss $w(s', Q)$, where $s' \in [0, s]$ is a spatial variable:

$$\frac{\partial f}{\partial s}(s, \Delta) = \int_0^\infty w(s, Q)[f(s, \Delta - Q) - f(s, \Delta)]dQ.$$ (4.86)

We use the following relationship to perform a Laplace transformation and solve for the general solution of the energy straggling distribution:

$$f(s, \Delta) = \frac{1}{2\pi i} \int_{-i\infty + \sigma}^{i\infty + \sigma} e^{\tau \Delta} \hat{F}(\tau, s) d\tau,$$ (4.87)

$$\hat{F}(\tau, s) = \int_0^\infty f(\Delta)e^{-\tau \Delta} d\Delta.$$ (4.88)
We multiply Eq. (4.86) by $e^{-\tau\Delta}$, integrate over $\Delta$, and apply Eq. (4.88)

$$e^{-\tau\Delta} \frac{\partial f(s, \Delta)}{\partial s} = e^{-\tau\Delta} \int_0^\infty w(s', Q)[f(s, \Delta - Q) - f(s, \Delta)]dQ,$$

(4.89)

$$\frac{\partial}{\partial s} \int_0^\infty e^{-\tau\Delta} f(s, \Delta)d\Delta = \int_0^\infty e^{-\tau\Delta} \int_0^\infty w(s', Q)[f(s, \Delta - Q) - f(s, \Delta)]dQd\Delta,$$

(4.90)

$$\frac{\partial}{\partial s} \hat{F}(s, \tau) = \int_0^\infty w(s', Q) \left\{ \int_0^\infty e^{-\tau\Delta}[f(s, \Delta - Q) - f(s, \Delta)]d\Delta \right\} dQ,$n

$$= \int_0^\infty w(s', Q) \left[ \hat{F}(s, \tau)e^{-\tau Q} - \hat{F}(s, \tau)d\Delta \right] dQ,$n

$$= -\hat{F}(s, \tau) \int_0^\infty w(s', Q)(1 - e^{-\tau Q})dQ. \quad (4.91)$$

We solve this first-order ODE and arrive at the solution of the form

$$\hat{F}(\tau, s) = \exp \left[ - \int_0^s \int_0^\infty w(s', Q)(1 - e^{-\tau Q})dQd\tau \right]. \quad (4.92)$$

We assume the probability of energy loss term $w(s', Q)$ to be piecewise-constant as a function of space $s'$:

$$w(s', Q) = \frac{2\pi e^4 N(s')Z(s')}{m_ec^2\beta^2} \frac{1}{Q^2}, \quad (4.93)$$

For a domain comprised of $n$ material types, the integral of Eq. (4.93) with respect to $s'$ can be expressed as a sum

$$\int_0^s w(s', Q)ds = \sum_n l_n w_n(Q), \quad (4.94)$$

$$w_n(Q) = \frac{2\pi e^4 N_n Z_n}{m_ec^2\beta^2} \frac{1}{Q^2}, \quad (4.95)$$

$$s = \sum_n l_n, \quad (4.96)$$
where \( l_n \) is the total length of material \( n \) within the step length \( s \). The solution is now in the following form:

\[
f(s, \Delta) = \frac{1}{2\pi i} \int_{i\infty+\sigma}^{i\infty+\sigma} \exp \left[ \tau \Delta - \sum_{n} l_n \int_{0}^{\infty} w_n(Q) (1 - e^{\tau Q}) dQ \right] d\tau.
\] (4.97)

Using the same approach as Landau, we evaluate the integral over \( w_n(Q) \) by splitting the integral over \( dQ \) at \( Q = Q_1 \) for low and high energy losses:

\[
\int_{0}^{\infty} w_n(Q) (1 - e^{-\tau Q}) dQ = \int_{0}^{Q_1} w_n(Q) (1 - e^{-\tau Q}) dQ + \int_{Q_1}^{\infty} w_n(Q) (1 - e^{-\tau Q}) dQ.
\] (4.98)

For the first term on the right-hand side, we use a first-order Taylor series expansion to approximate the exponential term \( \tau Q_1 \ll 1 \Rightarrow e^{-\tau Q} \approx 1 - \tau Q \) and use the well-known expression of Livingston and Bethe to account for shell effects for material \( n \):

\[
\tau \int_{0}^{Q_1} Qw_n(Q)dQ = \tau \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \ln \left( \frac{Q_1}{Q_1} \right),
\] (4.99)

where

\[
\ln(Q_n') = \ln \left[ \frac{(1 - \beta^2) I_n^2}{2m v^2} \right] + \beta^2,
\] (4.100a)

\[
I_n = Z_n I_0.
\] (4.100b)

Evaluating the second term on the right-hand side using u-substitution and Rutherford’s scattering cross section for material \( n \), we get

\[
\int_{Q_1}^{\infty} w_n(Q)(1 - e^{-\tau Q}) dQ = \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \int_{Q_1}^{\infty} \frac{1 - e^{-\tau Q}}{Q^2} dQ,
\]

\[
= \tau \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} [1 - \gamma - \ln(\tau Q_1)].
\] (4.101)
Combining the low and high energy loss integral terms and distance traveled in each material \( l_n \) yields

\[
\int_{0}^{\infty} w_n(Q)(1 - e^{-\tau Q})dQ = \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \left[ 1 - \gamma - \ln(\tau Q_n') \right],
\]

\[
\Rightarrow \sum_{n} l_n \int_{0}^{\infty} w_n(Q)(1 - e^{-\tau Q})dQ = \tau \sum_{n} \xi_n \left[ 1 - \gamma - \ln(\tau Q_n') \right],
\]

(4.102)

where

\[
\xi_n = \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} l_n.
\]

(4.103)

We apply the density effect correction factor \( \delta_n \) for material \( n \) in the same ad hoc manner as was done for the single material case and arrive at our solution of the energy loss straggling distribution for a stochastic mixture:

\[
f_L(s, \Delta) = \frac{1}{\xi} \int_{i\infty+\sigma}^{-i\infty+\sigma} \exp \left\{ \tau \Delta - \tau \sum_{n} \xi_n \left[ 1 - \gamma - \delta_n - \ln(\tau Q_n') \right] \right\} d\tau.
\]

(4.104)

We can conduct a transformation of variables \( f_L(s, \Delta)d\Delta = \phi(\lambda)d\lambda \), where \( u = \tau \xi \), which yields a universal function for a stochastic realization:

\[
f_L(s, \Delta) = \frac{1}{\xi} \phi(\lambda),
\]

(4.105a)

\[
\phi(\lambda) = \frac{1}{2\pi i} \int_{i\infty+\sigma}^{i\infty+\sigma} e^{u\ln(u)+u\lambda} du,
\]

(4.105b)

\[
\lambda = \frac{1}{\xi} \left\{ \Delta - \sum_{n} \xi_n \left[ 1 - \gamma - \delta_n - \ln \left( \frac{Q_n'}{\xi} \right) \right] \right\},
\]

(4.105c)

\[
\xi = \sum_{n} \xi_n.
\]

(4.105d)
4.3.2 Blunck & Leisegang

Blunck and Leisegang improved Landau’s distribution by using a second-order Taylor series expansion, \(1 - e^{-\tau Q} \approx 1 - \tau Q + (\tau Q)^2/2\), to approximate the exponential term in the small energy loss integral expression. They expressed their result as a convolution of Landau’s energy loss distribution with a Gaussian. For a stochastic mixture, the small energy loss term is

\[
\sum_{n}^{N} l_n \int_{0}^{\infty} w_n(Q)(1 - e^{-\tau Q})dQ = \sum_{n}^{N} l_n \int_{0}^{Q_1} w_n(Q) \left[ \tau Q - \frac{(\tau Q)^2}{2} \right] dQ \\
+ \sum_{n}^{N} l_n \int_{Q_1}^{\infty} w_n(Q)(1 - e^{-\tau Q})dQ,
\]

\[
= \tau \sum_{n}^{N} l_n \int_{0}^{Q_1} w_n(Q)QdQ - \frac{\tau^2}{2} \sum_{n}^{N} l_n \int_{0}^{Q_1} w_{n,1}(Q)Q^2dQ \\
+ \sum_{n}^{N} l_n \int_{Q_1}^{\infty} w_n(Q)(1 - e^{-\tau Q})dQ,
\]

where \(w_{n,1}(Q)\) is the probability of energy loss from distant collisions in material \(n\) and becomes less dominant at high kinetic energies \((w_{n,1}(Q) \approx 1/Q^\nu, \nu \approx 4 - 5)\) [17]. To evaluate the second-order term, \(w_{n,1}\) is approximated using a Dirac delta function at point \(1.5I_{s,n}\), similarly to Blunck and Leisegang, where \(I_{s,n}\) is the ionization potential of an electron in shell \(s\) of material \(n\) and 1.5 is an estimate from the width of the resonance curves. The expressions described in Eqs. (3.42) and (3.42c) are generalized for stochastic mixtures using
material index $n$:

$$\overline{Q}_n^q = \int_0^{Q_1} Q^2 w_{n,1}(Q) dQ,$$

$$w_{n,1}(Q) = \sum_s \frac{Q_{n,s} \delta(Q - 1.5I_{n,s})}{1.5I_{n,s}},$$

$$\overline{Q}_n = \sum_n \sum_s Q_{n,s} = \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \sum_n \sum_s R_{n,s} \frac{\ln \left[ \frac{2m v^2}{I_{n,s}(1 - \beta^2)} \right]}{Z_n},$$

where $R_{n,s}$ is the number of electrons of ionization potential $I_{n,s}$ in material $n$. The second-order term evaluates to be

$$\frac{\tau^2}{2} \sum_n^N l_n \int_0^{Q_1} Q^2 w_{n,1}(Q) dQ = \frac{\tau^2}{2} \sum_n^N l_n \overline{Q}_n^q,$$

$$= \frac{\tau^2}{2} \sum_n^N l_n \int_0^{Q_1} Q^2 \left[ \sum_s \frac{Q_{n,s} \delta(Q - 1.5I_{n,s})}{1.5I_{n,s}} \right] dQ$$

$$= \frac{\tau^2}{2} \sum_n^N l_n \left[ 1.5 \sum_{n,s} I_{n,s} Q_{n,s} \right],$$

$$= \frac{\tau^2}{2} \sum_n^N l_n \left\{ 1.5 \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \sum_{n,s} I_{n,s} \frac{R_{n,s}}{Z_n} \frac{\ln \left[ \frac{2m v^2}{I_{n,s}(1 - \beta^2)} \right]}{I_{n,s}(1 - \beta^2)} \right\},$$

$$= \frac{\tau^2}{2} \sum_n^N \xi_n \left\{ 1.5 \sum_{n,s} I_{n,s} \frac{R_{n,s}}{Z_n} \ln \left[ \frac{2m v^2}{I_{n,s}(1 - \beta^2)} \right] \right\}. \quad (4.108)$$

We now perform the Gaussian convolution, where the Gaussian has the following form:

$$g(r) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[ \frac{(r - r_0)^2}{2\sigma^2} \right], \quad (4.109)$$
and \( r_0 \) and \( \sigma^2 \) are the mean and variance. According to the convolution theorem for Fourier integrals, the following identities hold true:

\[
f^*(x) = \mathcal{F}^{-1}(\hat{f} \hat{g})(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{f}(\omega) \hat{g}(\omega) e^{i\omega x} d\omega, \tag{4.110a}
\]

\[
\hat{f}(\omega) = \mathcal{F}[f(x)] = \int_{-\infty}^{+\infty} f(x) e^{-i\omega x} dx, \tag{4.110b}
\]

\[
f(x) = \mathcal{F}^{-1}[\hat{f}(\omega)] = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{f}(\omega) e^{i\omega x} d\omega. \tag{4.110c}
\]

Beginning with Eq. (4.110a), we perform a convolution between Landau’s distribution for a stochastic mixture \( f_L(s, \Delta) \) and a Gaussian distribution, apply the Fourier transform of a Gaussian distribution Eq. (4.110b), and rearrange terms:

\[
f^*(s, \Delta) = \mathcal{F}^{-1}(\hat{f} \hat{g})(\Delta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{f}_L(s, \omega) \left[ \int_{-\infty}^{+\infty} g(x) e^{-i\omega x} dx \right] e^{i\omega \Delta} d\omega,
\]

\[
= \int_{-\infty}^{+\infty} g(x) \left[ \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{f}_L(s, \omega) e^{i\omega (\Delta - x)} d\omega \right] dx,
\]

\[
= \int_{-\infty}^{+\infty} f_L(s, \Delta - x) g(x) dx. \tag{4.111}
\]

We use the Gaussian distribution with a mean of \( x_0 = 0 \) and the second-order term for a region of multiple materials as the variance \( \sigma^2 = \sum_n l_n \overline{Q}^2_n \). This is analogous to the work of Blunck and Leisegang, who use the second-order term of a single material region \( L \overline{Q}^2 \) as
the variance:

\[
f^*(s, \Delta) = \int_{-\infty}^{\infty} f_L(s, \Delta - x)g(x)dx,
\]

\[
= \int_{-\infty}^{\infty} f_L(s, \Delta - x) \left[ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left( -\frac{(x - x_0)^2}{2\sigma^2} \right) \right] dx,
\]

\[
= \frac{1}{\sqrt{2\pi\sum_{n}^{N} l_n Q_n^2}} \int_{-\infty}^{\infty} f_L(s, \Delta - x) \exp\left( -\frac{x^2}{2\sum_{n}^{N} l_n Q_n^2} \right) dx.
\]  

(4.112)

Blunck and Leisegang numerically determined an approximate expression of \( \phi(\lambda) \) as the sum of Gauss functions, Eq. (3.45) and found the standard deviation for one material region using the second-order term of the small energy loss expression:

\[
b_{BL} = \frac{\sqrt{2\sigma^2}}{\xi} = \frac{\sqrt{2sQ^2}}{\xi}.
\]  

(4.113)

For a stochastic mixture, we similarly define the standard deviation for energy loss straggling in stochastic mixtures using the second-order term derived in Eq. (4.108):

\[
b_{BL} = \frac{\sqrt{2\sigma^2}}{\xi} = \frac{\sqrt{2\sum_{n}^{N} l_n Q_n^2}}{\xi}.
\]  

(4.114)

### 4.3.3 Chechin & Ermilova

Chechin and Ermilova conducted an error analysis as a result of neglecting higher-order moments [17] by including the third-order Taylor series term for the small energy loss term, \(1 - e^{-\tau Q} \approx 1 - \tau Q + (\tau Q)^2/2 - (\tau Q)^3/6\). We conduct the same analysis for stochastic media.
and begin by evaluating the integral over \( w_n(Q) \) for low energy losses \( Q \in [0, Q_1] \):

\[
\sum_n^N l_n \int_0^{Q_1} w_n(Q)(1 - e^{-\tau Q})dQ = \sum_n^N l_n \int_0^{Q_1} w_n(Q) \left[ \tau Q - \frac{(\tau Q)^2}{2} + \frac{(\tau Q)^3}{6} \right] dQ, 
\]

\[
= \tau \sum_n^N l_n \int_0^{Q_1} Qw_n(Q)dQ - \frac{\tau^2}{2} \sum_n^N l_n \int_0^{Q_1} Q^2w_{n,1}(Q)dQ 
+ \frac{\tau^3}{6} \sum_n^N l_n \int_0^{Q_1} Q^3w_{n,1}(Q)dQ. \tag{4.115}
\]

To evaluate the third-order term, we apply a similar analysis conducted by Blunck and Leisegang on the second-order term, where \( w_{n,1} \) is approximated using a Dirac delta function at point \( 1.5I_{n,s} \), shown in Eq. (4.107):

\[
\frac{\tau^3}{6} \sum_n^N l_n \int_0^{Q_1} Q^3w_{n,1}(Q)dQ = \frac{\tau^3}{6} \sum_n^N l_n \overline{Q_n^3},
\]

\[
= \frac{\tau^3}{6} \sum_n^N l_n \int_0^{Q_1} Q^3 \left[ \sum_s Q_{n,s} \delta(Q - 1.5I_{n,s}) \right] dQ
\]

\[
= \frac{\tau^3}{6} \sum_n^N l_n \left[ 1.5^3 \sum_s I_{n,s} \overline{Q_{n,s}} \right]
\]

\[
= \frac{\tau^3}{6} \sum_n^N l_n \left\{ 1.5^2 \frac{2\pi e^4 N_n Z_n}{m_c^2 \beta^2} \sum_s I_{n,s}^2 \frac{R_{n,s}}{Z_n} \ln \left[ \frac{2mv^2}{I_{n,s}(1 - \beta^2)} \right] \right\},
\]

\[
= \frac{\tau^3}{6} \sum_n^N \xi_n \left\{ 1.5^2 \sum_s I_{n,s}^2 \frac{R_{n,s}}{Z_n} \ln \left[ \frac{2mv^2}{I_{n,s}(1 - \beta^2)} \right] \right\}. \tag{4.116}
\]

In Blunck and Leisegang’s work, they define the mean energy loss per cm on a microscopic level, accounting for the excitation potential of each electron within a material \( n \). In Chechin’s work, a weighted-average of the excitation potential is used to express the mean
logarithmic excitation potential of matter, which is generalized to multiple materials

\[
\overline{Q_n} = \sum_s Q_{n,s} = \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \sum_s R_{n,s} \frac{Z_n}{Z_n} \ln \left( \frac{2mv^2}{I_{n,s}(1 - \beta^2)} \right),
\]

\[
= \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \sum_s R_{n,s} \ln \left( \frac{2mv^2}{(1 - \beta^2)} \right) - \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \sum_s R_{n,s} \ln(I_{n,s}),
\]

\[
= \frac{2\pi e^4 N_n Z_n}{m_e c^2 \beta^2} \ln \left( \frac{2mv^2}{I_n(1 - \beta^2)} \right),
\]

where

\[
\ln(I_n) = \sum_s \frac{R_{n,s}}{Z_n} \ln(I_{n,s}).
\]

Using a weighted-average of the excitation potential to preserve the mean logarithmic excitation potential of matter, as done by Chechin and Ermilova, the second-order term, Eq. (4.108), and third-order term, Eq. (4.116), simplify to

\[
\frac{\tau_2}{2} \sum_n I_n \overline{Q_n}^2 = \frac{\tau_2}{2} \sum_n \xi_n \left\{ 1.5 \sum_s I_{n,s} \frac{R_{n,s}}{Z_n} \ln \left( \frac{2mv^2}{I_{n,s}(1 - \beta^2)} \right) \right\},
\]

\[
= \frac{\tau_2}{2} \sum_n \xi_n I_n [\beta^2 - \ln(Q_n') + \ln(I_n)],
\]

\[
= \frac{\tau_2}{2} \sum_n \xi_n I_n \ln(a_n),
\]

(4.119a)

\[
\frac{\tau_3}{6} \sum_n I_n \overline{Q_n}^3 = \frac{\tau_3}{6} \sum_n \xi_n \left\{ 1.5^2 \sum_s I_{n,s}^2 \frac{R_{n,s}}{Z_n} \ln \left( \frac{2mv^2}{I_{n,s}(1 - \beta^2)} \right) \right\},
\]

\[
= \frac{\tau_3}{6} \sum_n \xi_n I_n^2 [\beta^2 - \ln(Q_n') + \ln(I_n)],
\]

\[
= \frac{\tau_3}{6} \sum_n \xi_n I_n^2 \ln(a_n),
\]

(4.119b)
where
\[ \ln(a_n) = \beta^2 - \ln(Q'_n) + \ln(I_n). \] (4.120)

This result shows that the AM approximation is preserved in the second-order and third-order term for a single realization.

We now derive the error term based on the analysis of Chechin using the relationship \( \tau_L \approx 1/\xi \), which comes from the integration region of significance. The estimated correction to the Landau formula for a stochastic mixture comes from the second-order low-energy loss term for a stochastic mixture and is of the order
\[ \eta_L \approx \tau_L^2 \sum_n \xi_n I_n \ln(a_n), \]
\[ = \frac{\sum_n \xi_n I_n \ln(a_n)}{\xi^2}. \] (4.121)

To estimate the correction to the Blunck-Leisegang formula for a stochastic mixture, we use the region of significance relationship in the form \( u^2 = (\tau \xi)^2 + O(\tau^2) \approx 1^2 \), where \( O(\tau^2) \) is the second-order term from the Taylor-series expansion:
\[ u^2 = (\tau \xi)^2 + \frac{\tau^2}{2} \sum_n \xi_n I_n \ln(a_n), \]
\[ 1 \approx \tau_B^2 \xi^2 + \tau_B^2 \sum_n \xi_n I_n \ln(a_n), \]
\[ 1 = \tau_B^2 \left( \xi^2 + \sum_n \xi_n I_n \ln(a_n) \right), \]
\[ \Rightarrow \tau_B = \frac{1}{\left( \sum_n \xi_n I_n \ln(a_n) + \xi^2 \right)^{1/2}}. \] (4.122)

Applying this relationship to the third-order term for a stochastic mixture results in the third-order correction to the Landau energy loss straggling distribution for a stochastic mixture.
mixture:

\[
\eta_B \approx \tau_B^3 \sum_n^N \xi_n I_n^2 \ln(a_n),
\]

\[
= \left[ \sum_n^N \xi_n I_n \ln(a_n) + \xi^2 \right]^{-\frac{3}{2}} \left( \sum_n^N \xi_n I_n^2 \ln(a_n) \right),
\]

\[
= \left( \sum_n^N \xi_n I_n^2 \ln(a_n) \right) \left( \sum_n^N \xi_n I_n \ln(a_n) \right)^{-\frac{3}{2}} \left[ 1 + \frac{\xi^2}{\sum_n^N \xi_n I_n \ln(a_n)} \right]^{-\frac{3}{2}},
\]

\[
= \frac{\sum_n^N \xi_n I_n^2 \ln(a_n)}{\left( \sum_n^N \xi_n I_n \ln(a_n) \right)^{\frac{3}{2}}} \left[ 1 + \frac{\xi^2}{\sum_n^N \xi_n I_n \ln(a_n)} \right]^{-\frac{3}{2}} .
\]

We use an analogous error expression as Seltzer [85] to provide a correction to our variance for a stochastic mixture:

\[
\sigma = \frac{b_{BL}}{1 + 3\epsilon_{CE}} .
\]

4.3.4 Ensemble-Average Energy Loss Straggling Distribution

For a stochastic domain, the condensed history algorithm requires that a new energy loss straggling distribution is computed at the beginning of each new substep length to account for the energy loss in the specific materials traversed in that substep. However, this can become computationally expensive. Here, we derive an ensemble-averaged energy loss straggling distribution for a binary, Markov process. If the length traversed in material 0 is known, Equations (4.104) and (4.112) can be written as a conditional probability function

\[
f(\Delta|l_0, s) = \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} \exp \left\{ \tau \Delta - \tau \xi_0 [1 - \gamma - \delta_0 - \ln(\tau Q_0')] - \tau \xi_1 [1 - \gamma - \delta_1 - \ln(\tau Q_1')] \right\} d\tau,
\]

\[
= \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} \exp \left\{ \tau \Delta - l_0 \frac{2\pi e^4 N_0 Z_0}{m_e c^2 \beta^2} [1 - \gamma - \delta_0 - \ln(\tau Q_0')] \right\} d\tau,
\]

\[
- (s - l_0) \frac{2\pi e^4 N_1 Z_1}{m_e c^2 \beta^2} [1 - \gamma - \delta_1 - \ln(\tau Q_1')] \right\} d\tau .
\]
and

\[ f^*(\Delta|l_0, s) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(\Delta - x|l_0, s)g(x)dx. \]  (4.126)

We can then integrate the joint probability density function over \( l_0 \) from 0 to \( s \) to get the ensemble-averaged probability density function for energy straggling:

\[ f^*(\Delta) = \int_0^s f^*(\Delta|l_0, s)f(l_0, s)dl_0, \]  (4.127)

where \( f(l_0, s) \) is the transit-length density for a binary Markovian material segment of length \( s \) that is traversed during an electron substep described in Eqs. (4.44).

### 4.4 Secondary Particle Production in Binary Markovian-Mixed Media

The production of secondary particles via hard collisions and bremsstrahlung emission in stochastic mixtures is handled in an analog manner at the end of each electron substep, and the sampling processes are largely similar to how the production of secondary particles are handled in a condensed history algorithm for a homogeneous background material. However, for a stochastic mixture, the event of a hard collision and bremsstrahlung emission are material-dependent. Therefore, an adequate mean free path that considers the transit-length of each material traversed by the electron must be used to properly compute the number of mean free paths for each substep. For a binary, Markovian-mixed segment of substep length \( s \), the expected mean free path is

\[ \lambda_i = \int_0^s f(l_0, s) \left[ \frac{l_0}{s} \lambda_{0,i} + \frac{s - l_0}{s} \lambda_{1,i} \right] dl_0, \]  (4.128a)

\[ \lambda_{n,i} = \frac{1}{N_n\sigma_{n,i}}, \]  (4.128b)
where \( i \) is the interaction index for a hard collision event \( hc \) or bremsstrahlung emission \( br \), \( N_n \) is the number density of material \( n \), and \( f(l_0, s) \) is the transit-length density for a binary Markovian material segment of length \( s \) described in Eqs. (4.44). For hard collisions, the cross section \( \sigma_{n, hc} \) of material \( n \) is computed using Eqs. (2.19b) and (2.22). For bremsstrahlung emission, the cross section \( \sigma_{n, br} \) of material \( n \) is computed using Eqs. (2.28). The probabilities of the interaction \( i \) occurring in material 0 and 1 are

\[
P_{0,i} = \frac{1}{\lambda_i} \int_0^s f(l_0, s) \frac{l_0}{s} \lambda_{0,i} dl_0, \tag{4.129a}
\]

\[
P_{1,i} = 1 - P_{0,i}. \tag{4.129b}
\]

Because the energy loss and angular deflection of the primary electron are accounted for in the multiple-scattering theories for a binary mixture, the energy and direction of the primary electron are not effected after a hard collision event. This is similar to how the energy loss and angular deflection of the primary electron are treated in a homogeneous background material. The energy and direction of the secondary electron is computed using the expressions described in Eqs. (2.23) and (2.19), respectively. In this work, hard collisions are sampled by decrementing the number of mean free paths, Eq. (3.62), to hard collision as the electron traverses the medium until a hard collision occurs as described in Section 3.4.1.

In the event of bremsstrahlung emission, the energy and direction of the primary electron are not accounted for in the multi-scatter energy loss straggling and angular deflection distributions. Similar to how this interaction is handled for a homogeneous background material, the scattering angle and energy of the photon and incident electron are sampled from tabulated data, which are derived from the radiative stopping power, Eq. (2.34). Bremsstrahlung photons are also sampled as described in Section 3.4.2, where the event of bremsstrahlung emission is sampled from the probability in Eq. (3.64), and in the event of a bremsstrahlung emission, the location of the event is uniformly sampled along the substep traveled.
4.5 Material-Dependent Energy Deposition in Binary Markovian-Mixed Media

The method for condensed history electron transport in stochastic media proposed in this work does not generate full material realizations. Therefore, geometric information is lost during particle transport. This section presents a novel methodology to approximate the energy deposition in each material. The total energy loss of an electron with initial energy $W$ after traversing a distance $s$ through some material $n$ is

$$\Delta E_n(W, s) = \int_0^s \frac{dE_n}{dx}(W) dx,$$  \hspace{1cm} (4.130)

where $dE(W)/dx$ is the stopping power. The mean stopping power of an electron traversing a length $s$ with initial energy $W$ in material $n$ is

$$\overline{dE_n}(W, s) = \frac{1}{s} \Delta E_n(W, s) = \frac{1}{s} \int_0^s \frac{dE_n}{dx}(W) dx,$$  \hspace{1cm} (4.131)

For a single step length $s$, where the electron traverses material 0 a distance of $l_0$ and material 1 a distance of $s - l_0$ in a binary mixture, the total energy loss of the electron can be approximated using the mean stopping power of each material in a random realization:

$$\Delta E(W, s|l_0) = \Delta E_0(W, s|l_0) + \Delta E_1(W, s|l_0),$$  \hspace{1cm} (4.132)

$$\Delta E_0(W, s|l_0) = l_0 \overline{dE_0}(W, s),$$  \hspace{1cm} (4.133)

$$\Delta E_1(W, s|l_0) = (s - l_0) \overline{dE_1}(W, s).$$  \hspace{1cm} (4.134)

In a binary, Markovian mixture, the mean stopping power of an electron traversing material $n$ and telegraph distribution are used to approximate the ensemble average energy fraction
4.6 Condensed History Algorithm in Binary Markovian-Mixed Media

This section explains how multi-scatter distributions, the number of particle interactions, and energy fraction deposition quantities were computed and implemented in a condensed history algorithm for photon-electron transport in binary Markovian-mixed media in this work. This method may be broken into three basic modules as depicted in Figure 4.2.

![Workflow of condensed history algorithm for photon-electron transport in binary Markovian-mixed media](image)

Figure 4.2: Workflow of condensed history algorithm for photon-electron transport in binary Markovian-mixed media

This method begins by precomputing data at start-up based on user-input material parameters (material mean chord lengths $\Lambda_0$ and $\Lambda_1$). In this work, this data was precomputed in Python 3.8, and numerical quadrature was used as the integration scheme throughout this work. Specifically, the function `quad` from the `integrate` package of the Python library

deposited in material 0:

$$\epsilon_0 = \frac{\int_0^s f(l_0, s) \Delta E_0(W, s|l_0) dl_0}{\int_0^s f(l_0, s) \Delta E(W, s|l_0) dl_0},$$

(4.135)
SciPy was used to perform integral calculations, which uses a Clenshaw-Curtis method with Chebyshev moments. This data is then used in the second module throughout particle transport. The code developed to precompute data is available in a repository\(^1\) hosted by Github. The code developed to perform particle transport is available in another repository\(^2\) hosted by Github. This tabulated data includes:

- step lengths, Eq. (3.1),
- ensemble-average angular deflection distributions, Eq. (4.84a),
- ensemble-average energy loss straggling distributions, Eq. (4.127),
- material fractions, which are used to compute mean number of interactions per substep during transport, Eq. (4.128),
- material-dependent energy deposition fractions, Eq. (4.135).

### 4.6.1 Computation of Step Lengths

In this work, electron step lengths are computed in a brute-force manner according to Algorithm 3. For this calculation, chord lengths of alternating materials are successively sampled until an 8.3% energy loss is achieved, and the total length of chord sampled is tallied. Energy loss calculations in this work are based on tabulated stopping power data printed from Table 85 of MCNP6.2 [109]. This is done numerous times, and the mean total length is computed to yield the electron step length for a given initial kinetic energy \(E\). The calculation for a single sample of an electron step length calculation is described in Algorithm 3. The associated energy loss from collisions is also tabulated for each step length to compute the mean collisional energy loss, which is used in the energy loss straggling distribution calculation.

\(^1\)https://github.com/emilyhvu0/ElectronMCTransport
\(^2\)https://github.com/emilyhvu0/StochasticPhotonElectronTransport
Algorithm 3 Calculation of electron step length in binary, Markovian-mixed media for initial kinetic energy $E$

1: Initialize total energy loss $\Delta E_{\text{tot}} = 0$
2: Initialize collisional energy loss $\Delta E_{\text{col}} = 0$
3: Initialize total length $s$
4: while $\Delta E_{\text{tot}} < 0.083E$ do
5:   Sample starting material $n$, Eq. (4.4)
6:   Sample chord length $\lambda_n$, Eq. (4.8), and associated total energy loss $\Delta E_{\text{tot},n}$
7:   if $\Delta E_{\text{tot}} + \Delta E_{\text{tot},n} > 0.083E$ then
8:     Truncate chord length $\lambda_n$ such that $\Delta E_{\text{tot}} + \Delta E_{\text{tot},n} = 0.083E$
9:     Accumulate chord length $s = s + \lambda_n$ and associated collisional energy loss $\Delta_{\text{col}} = \Delta_{\text{col}} + \Delta_{\text{col},n}$
10: Tally total length $s$ and collisional energy loss $\Delta E_{\text{col}}$

4.6.2 Computation of Ensemble Average Energy Loss Straggling Distributions

Once mean step lengths and the associated mean collisional energy losses are sampled, these quantities are used in the computation of the ensemble-average energy loss straggling distributions. To compute this distribution, first, the universal function $\phi_L(\lambda)$ described in Eq. (3.39a) is tabulated using numerical quadrature as the integration scheme [10] as described in Section 4.6:

$$\phi_L(\lambda) = \frac{1}{2\pi i} \int_{i\infty+\sigma}^{-i\infty+\sigma} e^{u\ln(u) + \lambda u} du,$$

$$\lambda = \frac{\Delta - \xi \left[ \ln \left( \frac{\xi}{Q'} \right) + 1 - \gamma - \delta \right]}{\xi}.$$

The integration of the distribution Eq. (4.127)

$$f^*(\Delta) = \int_0^s f^*(\Delta | l_0, s) f(l_0, s) dl_0$$

is then computed using numerical quadrature for energy losses $\Delta \in [0, E]$ up to the initial kinetic energy of the electron $E$. During this calculation, the parameter $l_0$ is used to compute the universal parameter $\lambda$ in Eq. (4.105c). This universal parameter $\lambda$ is then used to retrieve
the tabulated value \( \phi_L(\lambda) \) using a piecewise-linear interpolation scheme. The value \( \phi_L(\lambda) \) is then used to perform a convolution with a Gaussian using the corrected variance, described in Eq. (4.124) which is associated with \( l_0 \):

\[
\sigma = \frac{b_{BL}}{1 + 3\epsilon_{CE}}.
\]

Once this distribution has been calculated up to \( \Delta = E \), the distribution is truncated to preserve the mean collisional energy loss computed in Algorithm 3. This basic algorithm after the universal function \( \phi_L(\lambda) \) as been tabulated is described in Algorithm 4.

**Algorithm 4** Calculation of ensemble-average energy loss straggling distribution in binary, Markovian-mixed media for initial kinetic energy \( E \)

1: Initialize energy loss grid \( \Delta \in [0, E] \)
2: for each energy loss \( \Delta \in [0, E] \) do
3: Parameterize integration scheme using \( l_0 \) to solve Eq. (4.127)
4: for \( l_0 \in [0, s] \) do
5: Compute universal function \( \lambda \)
6: Compute corrected variance of Gaussian \( \sigma \)
7: Use piecewise-linear interpolation to find corresponding value \( \phi_L(\lambda) \) from tabulated data
8: Compute convolution using numerical quadrature
9: Truncate tail of distribution to preserve mean collisional energy loss \( \Delta E_{col} \)

### 4.6.3 Computation of Ensemble Average Angular Deflection Distributions

Substep lengths for \( m \) substeps are computed for each electron step length. These are used for the computation of the ensemble-average angular deflection distribution. The Legendre scattering moments \( G_\ell(s) \) of this distribution are computed, first, by using the \( N \)-point Gauss-Legendre quadrature formula, Eq. (3.16), as discussed on Section 3.2.1 to compute the inner integral with respect to \( \mu' \):

\[
\int_{-1}^{1} \frac{d\sigma^e_s}{d\Omega}(\mu') [1 - P_l(\mu)] d\mu \approx \sum_{n=1}^{N} w_n \frac{d\sigma^e_s}{d\Omega}(\mu_n) [1 - P_l(\mu_n)].
\]
In this work, we used $\ell = 501$ moments and $N = 101$ points. Then numerical quadrature is used to compute the integration involving the transit-length distribution with respect to $l_0$. Once these are computed for each order $\ell$, $F(s, \mu)$ may easily be computed for some grid $\mu \in [-1, 1]$. In this work, tabulated electron elastic scattering cross sections $d\sigma^e_s(\mu_i)/d\Omega$ were used for electron kinetic energies $E \in [1, 300]$ keV [76]. For $E > 300$ keV, electron elastic scattering cross sections were computed and tabulated using Eq. (2.14) in this work to account for additional physical effects discussed in Section 2.1.1:

$$\frac{d\sigma}{d\Omega} = \frac{Z^2e^2}{p^2v^2(1 - \mu + 2\eta)^2} \left[ \frac{(d\sigma/d\Omega)_{Mott}}{(d\sigma/d\Omega)_{Rath}} \right],$$

The algorithm to compute this ensemble-average angular deflection distribution is described in Algorithm 5.

**Algorithm 5** Calculation of ensemble-average angular deflection distribution in binary, Markovian-mixed media for initial kinetic energy $E$

1: Initialize Gauss-Legendre quadrature weights $w_i$ and roots $\mu_i$
2: Retrieve tabulated DCS values $d\sigma_s^e(\mu_i)/d\Omega$ at roots $\mu_i$
3: Initial grid $\mu \in [-1, 1]$
4: for each order $\ell$ do
5: Compute values of Legendre polynomial of order $\ell$ at roots $\mu_i$
6: Compute sum described in Eq. (3.16)
7: Use numerical quadrature to compute $G_\ell(s)$
8: Compute values of Legendre polynomial of order $\ell$ at grid values $\mu \in [-1, 1]$
9: Compute $F(s, \mu)$ described in Eq. (4.84a)

### 4.6.4 Computation of Secondary Particle Interaction Mean Free Paths

The mean number of bremsstrahlung photon and hard collision interactions are computed during transport according to the electron kinetic energy $E$ and substep length $s/m$ as a function of total length traveled. The mean free path $\lambda_{i,n} = 1/\Sigma_{i,n}(E)$ of the interaction $i$ in material $n$ is computed using the interaction cross section $\Sigma_{i,n}(E)$ at energy $E$. The number of interactions is then computed using the substep length and tabulated material fraction
\( \epsilon_l_0(s) \) of that length, which is used to weight the number of interactions in each material. For a length \( s \), the ensemble-average fraction of material 0 within some length \( s \) is

\[
\epsilon_l_0(s) = \frac{1}{s} \int_0^s f(l_0) l_0 dl_0,
\]

(4.136)

where the number of interactions \( k_i \) within some length \( s \) is

\[
k_i = \epsilon_l_0(s) s \lambda_{i,0} + [1 - \epsilon_l_0(s)] s \lambda_{i,1}.
\]

(4.137)

The ensemble-average material fractions \( \epsilon_l_0(s) \) for a prescribed length \( s \) are precomputed for lengths ranging from 0 to the maximum substep length \( s/m \) of the specified problem and is computed using numerical quadrature as the integration scheme as discussed in Section 4.6.

In this work, tabulated bremsstrahlung differential cross sections from MCNP6.2 [109] were used for the computation of bremsstrahlung photon mean free paths. This was done by modifying MCNP source code to print the bremsstrahlung DCS data that is precomputed at start-up. For hard collision mean free path calculations in this work, cross sections were computed using Eq. (2.19b):

\[
\sigma_{in,e}(\epsilon_c) = \frac{2\pi e^4}{m_c c^2 \beta^2 E} \left[ \frac{1}{\epsilon_c} - \frac{1}{1 - \epsilon_c} + \left( \frac{\kappa}{\kappa + 1} \right)^2 \frac{1}{2} \ln \left( \frac{1 - \epsilon_c}{\epsilon_c} \right) - \frac{2\kappa + 1}{(\kappa + 1)^2} \ln \left( \frac{1 - \epsilon_c}{\epsilon_c} \right) \right].
\]

4.6.5 Computation of Energy Deposition Fractions

The material-dependent energy deposition fraction in Eq. (4.135) is tabulated as a function of the electron initial kinetic energy:

\[
\epsilon_0 = \frac{\int_0^s f(l_0, s) \Delta E_0(W, s|l_0) dl_0}{\int_0^s f(l_0, s) \Delta E(W, s|l_0) dl_0}.
\]

This value is computed using numerical quadrature as the integration scheme as described in Section 4.6. During transport, this fraction is used at the end of each substep to compute the
portion of energy $\Delta$ (sampled from the ensemble-average energy loss straggling distribution) deposited in each material. For the set of material parameters investigated in this work, the computation of data in the first module required minutes of runtime to compute step lengths, angular deflection distributions, material fractions, and material-dependent energy deposition fractions. The computation of energy loss straggling distributions required days of computing and requires future work to improve this compute time.

4.6.6 Simulation of Particles

After the data has been precomputed and stored, the method moves on to the next module, where particles are transported using this tabulated data, described in Algorithm 6. In this work, particle transport algorithms were implemented in C++17. For electron transport in this work, the major step length and energy loss straggling distribution sampled at the beginning of each electron step are based on the initial energy of the electron at the beginning of the step and the nearest tabulated electron kinetic energy grid as a result of an 8.3% energy loss. In other words, the step lengths and energy loss straggling distributions used throughout transport are approximated based on this tabulated energy grid and are not based on the kinetic energy of the electron at the time of sampling. This introduces error into the transport solution since precomputed multi-scatter distributions are associated with precomputed step lengths that correspond to a specific kinetic energy.

To begin the condensed history algorithm, the kinetic energy and direction of the electron is initialized. An ensemble average, precomputed step length according to the electron kinetic energy is sampled based on the nearest tabulated electron kinetic energy. The corresponding ensemble average tabulated energy loss straggling distribution is sampled for the energy loss across this step length. The electron streams to the end of each substep. At the end of each substep, secondary particles are sampled and banked for transport later, a new angular deflection is sampled from the tabulated ensemble average multi-scatter distributions, and the preserved material probability is computed for the substep length traveled. This process
is repeated until the electron leaks the system or until its kinetic energy falls below the
cutoff energy of \( E = 1 \) keV. After all particle histories have been transported, the code
post-processes transport tallies to yield final transport calculations.

**Algorithm 6** Class I condensed history algorithm for stochastic media

1: Initialize electron
2: while \( E > 1 \) keV do
3: \hspace{1em} Sample major step length \( s \) according to nearest tabulated electron kinetic energy \( E \)
4: \hspace{1em} Sample energy loss per major step \( \Delta \) from tabulated ensemble-average energy loss
   straggling distribution \( F(\Delta) \)
5: \hspace{1em} Compute substep length \( \frac{s}{m} \) and mean energy loss per sub step \( \bar{\Delta} = \frac{\Delta}{t} \)
6: \hspace{1em} for each substep \( m \) do
7: \hspace{2em} Sample distance to boundary \( d_b \)
8: \hspace{2em} Stream particle to \( d = \min\{d_b, \frac{s}{m}\} \)
9: \hspace{2em} if \( d = \frac{s}{m} \) then
10: \hspace{3em} Deduct mean energy loss per sub step \( \bar{\Delta} \) from current electron energy \( E \)
11: \hspace{3em} Sample tabulated material length fraction \( \epsilon_{l_0} \) and compute distance traveled
   in each material \( l_0 = s\epsilon_{l_0} \) and \( l_1 = s - l_0 \) within substep
12: \hspace{3em} Compute number of bremsstrahlung photon and hard collision interactions \( k_i \).
13: \hspace{3em} if secondary particles are sampled then
14: \hspace{4em} Sample outgoing energy and direction
15: \hspace{4em} Store in particle bank
16: \hspace{3em} Compute preserved material probability, Eq. (4.2), at end of substep
17: \hspace{3em} Sample angular deflection \( \mu \) from tabulated ensemble-average angular deflec-
   tion distribution \( F(\mu) \)
18: \hspace{3em} if \( E < 1 \) keV then
19: \hspace{4em} Deposit electron energy \( E \)
20: \hspace{4em} Break
21: \hspace{3em} else
22: \hspace{4em} Terminate electron
23: \hspace{4em} Break
24: \hspace{2em} Simulate random walk of produced photons and secondary electrons
CHAPTER 5

Results and Analysis

5.1 Verification of Multiple-Scattering and Secondary Particle Production for Binary Markovian Mixtures

This section discusses how (i) the angular deflection and energy loss straggling multiple-scattering distribution generalized for binary, Markovian-mixed media, (ii) the production of secondary particles for binary, Markovian-mixed media, and (iii) material-dependent energy deposition, introduced in Chapter 4, were verified. This verification was conducted by computing the ensemble average distributions and quantities derived in Chapter 4 and comparing these results against the distributions and quantities computed and averaged over explicit material realizations.

5.1.1 Verification Problem Parameters

Here, results were produced for binary Markovian mixtures of carbon and lead, chosen because of their large difference in electron density. Table 5.1 provides the problem parameters of four material mixing configurations investigated in this section of carbon and lead material properties, indexed at 0 and 1 respectively. Two of these configurations are limiting cases.

- Case a: \( \Lambda_0 = \Lambda_1, \Lambda_0, \Lambda_1 < s \), we expect the ensemble average distribution to agree
with the Monte Carlo mean distribution.

- Case b: $\Lambda_0 < \Lambda_1$, $\Lambda_0, \Lambda_1 < s$, we expect the ensemble average distribution to agree with the Monte Carlo mean distribution and tend toward the pure lead distribution compared to Case a.

- Case c: $\Lambda_0, \Lambda_1 \ll s$, we expect the ensemble average distribution to agree with the distribution computed using an AM approximation.

- Case d: $\Lambda_0 \ll \Lambda_1$ and $\Lambda_0 \ll s$, we expect the ensemble average distribution to agree with the distribution computed for a pure lead segment.

Table 5.1: Material properties and chord lengths of carbon and lead for each case

<table>
<thead>
<tr>
<th>$n$</th>
<th>$Z$</th>
<th>$M$</th>
<th>$\rho$</th>
<th>Mean Chord Length $\Lambda_n$ [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$a$</td>
</tr>
<tr>
<td>0</td>
<td>6</td>
<td>12</td>
<td>2.2</td>
<td>$5 \times 10^{-6}$</td>
</tr>
<tr>
<td>1</td>
<td>82</td>
<td>207</td>
<td>11.3</td>
<td>$5 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

Ensemble average energy loss straggling distributions [100] as defined in Eq. (4.127), ensemble average angular deflection distributions [99] with coefficients defined in Eq. (4.84a), the mean free paths and material probabilities of secondary photon and electron production, as defined in Eqs. (4.128) and (4.129), and material-dependent energy deposition fractions defined in Eq. (4.135) are benchmarked against the mean distributions and values of random, fully generated, binary Markovian mixtures. These mean benchmark results presented in this section were produced using $10^5$ binary Markovian-mixed realizations of step and substep length $s = 10^{-5}$ cm by successively sampling exponentially distributed material chord lengths beginning with material 0. The integrals derived in Eq. (4.127) and Eq. (4.84a) of Chapter 4 were evaluated using numerical quadrature, as described in Section 4.6, to produce the results presented in this section.
5.1.2 Step Size and Mean Energy Loss

The mean step size of an electron with initial energy $E_{m-1}$ and collisional energy loss $\Delta E = E_{m-1} - E_m$ for a stochastic mixture was computed by, first, successively sampling material chord lengths and tallying the energy loss for each chord length until an 8.3% energy loss was achieved. This routine was executed 1000 times, and the average total length sampled was taken as the mean step size of an electron for initial energy $E_{m-1}$. Then, to compute the mean collisional energy loss, the collisional energy loss of each material chord within each of these mean step sizes was tallied. Figure 5.1 shows the mean total path length computed as a function total energy (left) and computed mean collisional energy as a function of mean total path length (right) for pure carbon, pure lead, and each case using initial material 0.

Figure 5.1: Monte Carlo mean range as a function of initial kinetic energy (left) and Monte Carlo mean collisional energy as a function of Monte Carlo mean range (right) of pure carbon, pure lead, and each case using initial material 0.

5.1.3 Energy Loss Straggling Distribution Verification

Figure 5.2 shows the energy loss straggling distribution for $\beta = 0.8$ of a step length $s = 10^{-5}$ cm of pure lead, pure carbon, an AM approximation, the ensemble average, and
Figure 5.2: Pure carbon, pure lead, Atomic Mix approximation, ensemble average, and Monte Carlo mean energy loss straggling distributions for each case using a step length of $10^{-5}$ cm.

Monte Carlo mean for cases a-d described in Table 5.1. For cases a and b in Figure 5.2, the computed ensemble average distributions agree with the Monte Carlo mean benchmark solutions. For cases c and d in Figure 5.2, the computed ensemble average distributions agree with the AM approximation and pure lead distribution, respectively, as well as the respective Monte Carlo mean benchmark solution. These results demonstrate that, for the set of benchmark parameters described in Table 5.1, the ensemble average energy loss distribution derived in Eq. (4.127) of Chapter 4 agrees with the Monte Carlo mean energy loss distribution of many stochastic material realizations derived in Eq.(4.125) for the limiting cases of a pure material and atomically homogenized materials, as well as the regime in between.
5.1.4 Angular Deflection Distribution Verification

Figure 5.3: Pure carbon, pure lead, atomic mix approximation, ensemble average, and Monte Carlo mean angular deflection distributions for each case using a substep length of $10^{-5}$ cm for scattering cosine $\mu \in [0.75, 1.0]$ and probabilities 0.0 to 0.25.

Figure 5.3 shows angular deflection distributions using an incoming electron kinetic energy $E = 0.5$ MeV and a substep length $s = 10^{-5}$ cm. For cases a-d described in Table 5.1, angular deflection distribution calculations were made for a substep length of pure lead, pure carbon, an AM approximation, the ensemble average, and the Monte Carlo mean. Because the angular deflection distributions are highly forward peaked, Figure 5.3 shows the scattering cosine $\mu \in [0.75, 1.0]$ and probabilities 0.0 to 0.25 for ease of comparison. Similar to the verification results for the ensemble energy loss straggling distributions, for this set of benchmark parameters, the computed ensemble average distributions agree with the Monte Carlo mean benchmark solutions. Additionally, the computed ensemble average angular deflection distribution for cases c and d agree with the AM approximation and pure lead distribution,
respectively. These results demonstrate that, for the set of benchmark parameters described in Table 5.1, the ensemble average angular deflection distribution derived in Eq. (4.84a) of Chapter 4 agrees with the Monte Carlo mean energy loss distribution of many stochastic material realizations derived in Eq. (4.84a) for the limiting cases of a pure material and atomically homogenized materials, as well as for the cases in which the material mean chord lengths are of the same length-scale as the substep length.

5.1.5 Hard Collision Electron Verification

Figure 5.4: Pure carbon, pure lead, ensemble average, and Monte Carlo mean hard collision mean free paths for each case as a function of initial kinetic energy

Figures 5.4 and 5.5 show the mean free path and probability of a hard collision event occurring in material 0, respectively, in a substep length corresponding to an 8.3% energy loss
Figure 5.5: Pure carbon, pure lead, ensemble average, and Monte Carlo mean probability of hard collision occurring in material 0 for each case as a function of initial kinetic energy of the initial energy (Figure 5.1) of pure lead, pure carbon, an atomic mix approximation, the ensemble average, and Monte Carlo mean for cases a-d as a function of initial electron kinetic energy for a substep beginning in material 0. Figures 5.4 and 5.5 demonstrate that the Monte Carlo mean results agree with the computed ensemble average mean free paths and probability of a hard collision event occurring in material 0, described in Eq. (4.128) and Eq. (4.129), respectively, for each case described in Table 5.1. In addition, for cases c and d, the AM approximation solution is shown to be a good approximation throughout the entire energy range investigated, $E \in [0.001, 10]$ MeV.

In Figure 5.5, the ensemble average solution converges towards the AM approximation solution as the initial electron kinetic energy increases. This is because, as the kinetic energy
of the electron increases, the electron is able to travel a larger distance to lose 8.3% of its kinetic energy, and therefore, the larger substep length $s$ becomes orders of magnitude greater than the mean chord lengths such that the AM approximation becomes a valid approximation.

5.1.6 Bremsstrahlung Photon Emission Verification

![Figure 5.6](image)

Figure 5.6: Pure carbon, pure lead, ensemble average, and Monte Carlo mean bremsstrahlung emission mean free paths for each case as a function of initial kinetic energy

Figures 5.6 and 5.7 show the mean free path and probability of a bremsstrahlung photon emission occurring in material 0, respectively, in a substep length corresponding to an 8.3% energy loss of the initial energy (Figure 5.1) comprised of pure lead, pure carbon, an AM approximation, the ensemble average, and Monte Carlo mean for cases a-d as a function of
Figure 5.7: Pure carbon, pure lead, ensemble average, and Monte Carlo mean probability of 
bremsstrahlung emission occurring in material 0 for each case as a function of initial kinetic 
energy beginning in material 0. Similar to Figures 5.4 and 5.5, Figures 5.6 
and 5.7 demonstrate that the Monte Carlo mean results agree with the computed ensemble 
average results and demonstrate that the Monte Carlo mean results agree with the computed 
ensemble average mean free paths and probability of a bremsstrahlung photon emission 
occurring in material 0, described in Eq. (4.128) and Eq. (4.129), respectively, for each case 
described in Table 5.1. Additionally, the AM approximation solution is shown to be a good 
approximation throughout the entire energy range investigated, $E \in [0.001, 10]$ MeV, for 
cases c and d. Similar to Figure 5.5, the ensemble average solution in Figure 5.7 converges 
towards the AM approximation as the initial kinetic energy increases because the step size $s$ 
becomes orders of magnitude greater than the mean chord lengths at greater kinetic energies.
5.1.7 Material-Dependent Energy Deposition Verification

Figure 5.8: Pure carbon, pure lead, ensemble average, and Monte Carlo mean energy deposition in material 0 for each case as a function of initial kinetic energy

Figures 5.8 and 5.9 show the mean energy deposited in material 0 and mean energy fraction deposited in material 0, respectively, in a substep length corresponding to an 8.3% energy loss of the initial energy (Figure 5.1) of pure lead, pure carbon, an AM approximation, the ensemble average, and Monte Carlo mean for cases a-d as a function of initial kinetic energy beginning in material 0. Figures 5.8 and 5.9 demonstrate that the Monte Carlo mean results agree with the compute ensemble average energy deposition, described in Eq. (4.132), and ensemble average energy deposition fraction, described in Eq (4.135), for each case described in Table 5.1.
5.2 Validation of Condensed History Model for Stochastic Media

Here, we validate our condensed history code developed for binary, Markovian-mixed media, which we call the Stochastic Mixture Accounted Condensed History Electron (SMACHE) method (pronounced “smash”). To the knowledge of the author, benchmark quality experimental results have not been published for electron transport problems in stochastic media. In this work, SMACHE was compared against methods that have been validated with experimental results for pure problems, namely the single-scatter approach, and its ability to reproduce results of existing methods was evaluated.

To validate SMACHE, we produce mean leakage rates and material-dependent energy deposition results and compare these results against MCNP6 benchmark results that were
produced using a single-scatter (SS) and condensed history (CH) method on problems for which the AM approximation is not a good approximation. These benchmark results were produced using 50 full material realizations, which were generated using the method of successively sampling exponentially distributed chord lengths of alternating material types as described in Section 4.1.2 and $10^6$ histories.

In this section, we discuss the problem parameters and test cases investigated in this work. We provide transport results for single-region slab problems and multi-region slab problems, an accuracy comparison of these results against benchmark values, and we demonstrate a novel capability of quantifying material-dependent energy deposition in binary, Markovian mixtures using SMACHE.

5.2.1 Validation Problem Parameters

Transport results of electron beam and photon beam source problems with respectively source energies $E_{e^-} = 0.1$ MeV and $E_{\gamma} = 10$ MeV were produced for single-region and multi-region slabs composed of pure materials and binary Markovian mixtures. For multi-region problems, a single interface located in the middle of the slab is investigated. The materials considered in this section are carbon, nitrogen (air), iron, and lead. We note that, in this section, carbon is always denoted as material 0 in mixtures.

These materials were chosen to examine SMACHE’s ability to accurately model photon-electron transport problems in a binary stochastic mixture of materials with void and varying differences in atomic number $Z$. Table 5.2 provides the properties of each of the materials investigated in this work.

Table 5.3 provides the mean chord lengths used for a pure slab of each material denoted as “C,” “N,” “Fe,” and “Pb” for pure carbon, pure nitrogen, pure iron, and pure lead, respectively, as well as the mean chord lengths of material mixing configurations used for a binary stochastic mixture denoted as “C-N”, “C-Fe”, and “C-Pb” for a stochastic mixture between carbon and nitrogen, carbon and iron, and carbon and lead, respectively. These
Table 5.2: Material properties of carbon, nitrogen, iron, and lead

<table>
<thead>
<tr>
<th>Material</th>
<th>Z</th>
<th>M</th>
<th>ρ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>6</td>
<td>12</td>
<td>2.2</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7</td>
<td>14</td>
<td>0.00125</td>
</tr>
<tr>
<td>Iron</td>
<td>26</td>
<td>56</td>
<td>7.874</td>
</tr>
<tr>
<td>Lead</td>
<td>82</td>
<td>207</td>
<td>11.3</td>
</tr>
</tbody>
</table>

Material combinations were chosen based on the material atomic number $Z$ to demonstrate how SMACHE may perform on applications with mixtures of similar differences in $Z$. For example, the mixture C-N is analogous to the make-up of tissue commonly found in medical applications, which can be comprised of carbon and void. The mixture of a high $Z$ and low $Z$ material such as in “C-Pb” is representative of ICF type problems where a laser rapidly compresses a fuel pellet, which may result in high $Z$ materials mixing with hydrogen because of Rayleigh-Taylor instabilities.

In addition, this work investigates the test case of a binary, Markovian mixture in which the first material type at the boundary is known. Specifically, a binary Markovian mixture between carbon and iron where the material type at the boundary is always carbon is investigated for a single-slab region, denoted as “C-Fe $P_0(0) = 1$.” The mean chord lengths provided in Table 5.3 were selected to be less than the electron range in each material for the respective source energy to ensure that the electron traverses multiple stochastic material zones within a step.

The accuracy of SMACHE is demonstrated on single-region slab problems composed of either a pure material or a binary, Markovian mixture. The accuracy of SMACHE is also demonstrated for multi-region slab problems having an interface located in the middle of the slab $x = L/2$. This interface creates two regions, each composed of either a homogeneous pure material or a binary, Markovian mixture. For example, “C|Pb” denotes a multi-region slab where the first half of the slab $0 \leq x \leq L/2$ is carbon and the last half of the slab $L/2 \leq x \leq L$ is lead. Another example is “C-Fe|C-Pb,” which denotes a multi-region slab.
Table 5.3: Mean chord lengths of pure materials and binary stochastic mixtures for electron source problems of $E_{e^-} = 0.1$ MeV and photon source problems of $E_\gamma = 10$ MeV

<table>
<thead>
<tr>
<th>Case</th>
<th>$E_{e^-} = 0.1$ MeV</th>
<th>$E_\gamma = 10$ MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Lambda_0$ [cm] $\Lambda_1$ [cm]</td>
<td>$\Lambda_0$ [cm] $\Lambda_1$ [cm]</td>
</tr>
<tr>
<td>C</td>
<td>1.0 0.0</td>
<td>1.0 0.0</td>
</tr>
<tr>
<td>N</td>
<td>1.0 0.0</td>
<td>1.0 0.0</td>
</tr>
<tr>
<td>Fe</td>
<td>1.0 0.0</td>
<td>1.0 0.0</td>
</tr>
<tr>
<td>Pb</td>
<td>1.0 0.0</td>
<td>1.0 0.0</td>
</tr>
<tr>
<td>C-N</td>
<td>0.001 0.001</td>
<td>0.1 0.1</td>
</tr>
<tr>
<td>C-Fe</td>
<td>0.001 0.001</td>
<td>0.1 0.1</td>
</tr>
<tr>
<td>C-Pb</td>
<td>0.001 0.001</td>
<td>0.1 0.1</td>
</tr>
</tbody>
</table>

where the first half of the slab $0 \leq x \leq L/2$ is a binary Markovian mixture of carbon and iron and the the last half of the slab $L/2 \leq x \leq L$ is a binary Markovian mixture of carbon and lead. The slab length and interface locations for each source energy problem investigated is provided in Table 5.4.

Table 5.4: Length $L$ of slab and location of interface $0 \leq x \leq L$ for single-region and multi-region slab for electron source problems $E_{e^-} = 0.1$ MeV and photon source problems of $E_\gamma = 10$ MeV

<table>
<thead>
<tr>
<th>Slab</th>
<th>$E_{e^-} = 0.1$ MeV</th>
<th>$E_\gamma = 10$ MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$L$</td>
<td>$x$</td>
</tr>
<tr>
<td>Single-Region</td>
<td>0.1</td>
<td>none</td>
</tr>
<tr>
<td>Multi-Region</td>
<td>0.01</td>
<td>0.005</td>
</tr>
</tbody>
</table>

To evaluate the accuracy of the mean electron and photon leakage rates as well as the material-dependent electron energy deposition results produced by SMACHE, the relative error is computed by comparing SMACHE results against benchmark results produced by MCNP6 using a SS and CH approach. The relative error is

$$E_R = \frac{x_{\text{approx}} - x}{x}, \quad (5.1a)$$

where $x$ is the mean benchmark value and $x_{\text{approx}}$ is the mean value produced by SMACHE.
The statistical uncertainty of the relative error is propagated, yielding

\[ U_{ER} = \sqrt{\left( \frac{U_{\text{approx}}}{x} \right)^2 + \left( \frac{x_{\text{approx}} U}{x^2} \right)^2}, \]  

(5.1b)

where \( U_{\text{approx}} \) is the statistical uncertainty of the mean value produced by SMACHE and \( U \) is the benchmark statistical uncertainty value. The mean absolute relative error computed in this section is

\[ \text{Mean}|E_R| = \frac{1}{N} \sum_i |E_{R_i}|, \]  

(5.1c)

where \( E_{R_i} \) is the relative error of case \( i \). In this work, results were produced with SMACHE using 10 substeps per step length, \( 5 \times 10^5 \) histories for \( E_{e^-} = 0.1 \) MeV electron source problems, and \( 10^5 \) histories for \( E_\gamma = 1 \) MeV photon source problems. In SMACHE, photons were transported assuming the AM approximation because of the large photon mean free path compared to the material mean chord lengths investigated in this work.

### 5.2.2 Single-Region Slab Results

For a single-region slab, infinite in the Cartesian coordinate directions \( y \) and \( z \), three types of problems are investigated:

- **Pure**: The background material of the slab is a singular, uniform material. In this work, the pure materials investigated are carbon (C), nitrogen (N), iron (Fe), and lead (Pb).

- **Mixed**: The background material of the slab is a region composed of a binary Markov mixture. In this work, the binary Markov mixtures investigated are mixtures of carbon and nitrogen (C-N), carbon and iron (C-Fe), and carbon and lead (C-Pb).

- **Mixed with first material known**: The background material of the slab is a region composed of a binary Markov mixture, where the material at the surface is known.
In this work, we investigate a carbon and iron mixture in which the first material is always carbon (C-Fe $P_0(0) = 1$).

In this section, we (i) present the mean leakage results and material-dependent energy deposition results for each single-region slab problem investigated, and (ii) provide an accuracy assessment on SMACHE compared to SS and CH benchmark results. Though we expect the error of SMACHE results compared to SS results to be greater than the error of SMACHE results compared to CH results, we report this comparison in this section to provide an evaluation of the accuracy of SMACHE compared to physically correct results.

5.2.2.1 Mean Particle Leakage Results

In Tables 5.5 and 5.6 are the mean photon and electron reflectance and transmittance rates, respectively, for each problem investigated for a single-region slab, where the statistical error on the last digit is provided in parenthese. The relative error of the mean photon and electron reflectance and transmittance rates produced by SMACHE compared to SS and CH benchmark results for these problems are provided in Table 5.7. The leakage rates and relative error of the pure nitrogen case produced using an electron source are excluded from these tables because these values were statistically insignificant. In Table 5.7, “–” denotes an undefined relative error and is a result of either a zero value benchmark result or a comparison of statistically insignificant values. For select cases where the CH relative error is relatively high because of a small mean benchmark value, the absolute error is reported in Table 5.8 to provide a sense of the statistical insignificance of the result.

5.2.2.2 Material-Dependent Electron Energy Deposition Results

Table 5.9 provides the total mean material-dependent electron energy deposition for each problem investigated for a single-region slab, and the relative error of SMACHE results compared to SS and CH benchmark results are provided in Table 5.10. We note that in Table 5.10, the absolute value of the relative error of the energy deposition in the pure
nitrogen case for a photon source problem is greater than one. For these cases, the absolute error of SMACHE results compared to the SS and CH benchmarks are $-2(1) \times 10^{-8}$ MeV and $6(1) \times 10^{-9}$ MeV, respectively.

SMACHE does not accurately compute the material-dependent electron energy deposition in nitrogen in the C-N mixture. This error may arise from several causes. First, this error could be due to the approximation made in Eq. (4.131), where the energy loss rate is assumed to be constant across a step length. More error may be introduced for a material like nitrogen with a density of 0.00125 g/cm$^3$ because of the significantly larger step size nitrogen has at this density to achieve an 8.3% energy loss. Additional error may arise from the fact that the transit length distribution derived in Eqs. (4.44) does not retain the order of materials in which the electron travels through. Additionally, error may also be introduced at the step level of the condensed history algorithm in which the step length and sampled energy loss straggling distribution is based on the nearest tabulated kinetic energy to the initial energy of the electron at the beginning of the step.

The capability to compute material-dependent energy deposition distributions within a stochastic mixture using SMACHE is demonstrated on the single-region stochastic mixtures outlined in Table 5.3. The material-dependent distributions as a function of slab depth of the electron energy deposition linear density for the $E_{\text{e}^-} = 0.1$ MeV electron beam source problems and $E_{\gamma} = 1$ MeV photon beam source problems are shown in Figure 5.10 and Figure 5.11, respectively, and agree with the general behavior of the CH benchmark energy deposition distributions.

5.2.2.3 Summary of SMACHE Accuracy on Single-Region Slab Problems

Using the computed relative errors in Tables 5.7 and 5.10, we find the mean absolute relative error of SMACHE compared to SS and CH benchmark results for mean photon and electron reflectance and transmittance rates as well as mean material-dependent electron energy deposition, which are provided in Table 5.11. These values show that, on average
Figure 5.10: Material-dependent electron energy deposition linear density distributions of $E_{e^-} = 0.1$ MeV electron beam source problems in binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary for the single-region benchmark problems investigated in this work, SHACHE performs best on electron leakage results when compared to the CH benchmark results as opposed to SS benchmark results, with roughly a mean absolute relative error of 5-10% for CH comparisons and 8-19% for SS comparisons. When excluding the electron energy deposited in nitrogen in the carbon-nitrogen (C-N) case for a photon beam source, we highlight that SMACHE is able to achieve a 15.0% average absolute relative error compared to SS benchmark results and a 13.6% average absolute relative error compared to CH benchmark results on material-dependent electron energy deposition calculations.
5.2.3 Multi-Region Slab Results

For a multi-region slab, infinite in the Cartesian coordinate directions $y$ and $z$, we investigate problems with an interface at $x = L/2$. We investigate two types of problems for which each region is:

- Pure: The background material regions are each composed of a pure, uniform material. The first half of the slab $0 \leq x \leq L/2$ is one pure material and the last half of the slab $L/2 \leq x \leq L$ is a different pure material. The material combinations of carbon in the first half of the slab and nitrogen, iron, and lead in the last half of the slab (C|N, C|Fe,
C|Pb, respectively) as well as nitrogen, iron, and lead in the first half of the slab and carbon in the last half of the slab (N|C, Fe|C, Pb|C, respectively) are investigated.

- Mixed: The background material regions are each composed of a binary Markov mixture. The first half of the slab $0 \leq x \leq L/2$ is one binary Markov mixture and the last half of the slab $L/2 \leq x \leq L$ is a different binary Markov mixture. The material combinations of a carbon and iron mixture in the first half of the slab and a carbon and lead mixture in the last half of the slab and visa versa (C-Fe|C-Pb and C-Pb|C-Fe, respectively) are investigated.

In this section, we (i) present the mean leakage results and material-dependent energy deposition for each multi-region problem investigated, and (ii) provide an accuracy assessment on SMACHE compared to SS and CH benchmark results.

### 5.2.3.1 Mean Particle Leakage Results

In Tables 5.12 and 5.13 are the mean photon and electron reflectance and transmittance rates, respectively, for each problem investigated for a multi-region slab. The relative error of the mean photon and electron reflectance and transmittance rates produced by SMACHE compared to SS and CH benchmark results are provided in Table 5.14. Similar to Table 5.7, an undefined relative error “–” in this table is a result of a zero value benchmark result or a comparison of statistically insignificant values. For select cases where the relative error is relatively high, the absolute error is also reported in Table 5.15.

### 5.2.3.2 Material-Dependent Electron Energy Deposition Results

Table 5.16 reports the total mean material-dependent electron energy deposition results for each problem investigated for a multi-region slab, and the relative error of SMACHE results compared to SS and CH benchmark results are provided in Table 5.17. Absolute error values for select cases with relatively high CH relative errors are presented in Table 5.18.
These results show that, for this set of benchmark problems, more error is generally introduced in the material-dependent electron energy deposition results compared to the single-region problems investigated in this paper. This is because of the additional approximations in energy loss and angular deflection that introduced into the particle track when truncating the electron substep length at an internal interface crossing in the multi-region slab.

5.2.3.3 Summary of SMACHE Accuracy on Multi-Region Slab Problems

Using the computed relative errors in Tables 5.14 and 5.10, the average relative error of SMACHE compared to SS and CH benchmark results for mean photon and electron reflectance and transmittance rates as well as mean material-dependent electron energy deposition are computed and provided in Table 5.19. These values show that, on average for the multi-region benchmark problems investigated, SMACHE performs best on electron reflectance rates compared to electron transmittance rates.
Table 5.5: Mean photon and electron reflectance rates of $E_{\gamma} = 0.1$ MeV electron beam source problems in a $L = 0.1$ cm single-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 1$ cm single-region slab of pure materials, binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary.

<table>
<thead>
<tr>
<th>Case</th>
<th>Particle</th>
<th>$E_{e^-} = 0.1$ MeV, $L = 0.1$ cm</th>
<th>Reflectance</th>
<th>SMACHER</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>SS</td>
<td>CH</td>
<td>SMACHER</td>
</tr>
<tr>
<td>C</td>
<td>$\gamma$</td>
<td>$1.17(3) \times 10^{-3}$</td>
<td>$1.21(3) \times 10^{-3}$</td>
<td>$1.18(5) \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.46(2) \times 10^{-2}$</td>
<td>$3.94(2) \times 10^{-2}$</td>
<td>$3.66(3) \times 10^{-2}$</td>
</tr>
<tr>
<td>Fe</td>
<td>$\gamma$</td>
<td>$1.16(1) \times 10^{-2}$</td>
<td>$1.10(1) \times 10^{-2}$</td>
<td>$1.07(1) \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$2.868(5) \times 10^{-1}$</td>
<td>$2.515(5) \times 10^{-1}$</td>
<td>$2.519(6) \times 10^{-1}$</td>
</tr>
<tr>
<td>Pb</td>
<td>$\gamma$</td>
<td>$1.07(1) \times 10^{-2}$</td>
<td>$7.70(9) \times 10^{-3}$</td>
<td>$7.8(1) \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.366(5) \times 10^{-1}$</td>
<td>$4.877(5) \times 10^{-1}$</td>
<td>$5.8(7) \times 10^{-1}$</td>
</tr>
<tr>
<td>C-N</td>
<td>$\gamma$</td>
<td>$1.19(1) \times 10^{-3}$</td>
<td>$1.78(5) \times 10^{-3}$</td>
<td>$1.18(5) \times 10^{-3}$</td>
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<tr>
<td></td>
<td>$e^-$</td>
<td>$5.45(2) \times 10^{-2}$</td>
<td>$3.85(7) \times 10^{-2}$</td>
<td>$4.27(3) \times 10^{-2}$</td>
</tr>
<tr>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$9.8(3) \times 10^{-3}$</td>
<td>$9.5(3) \times 10^{-3}$</td>
<td>$9.0(1) \times 10^{-3}$</td>
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<tr>
<td></td>
<td>$e^-$</td>
<td>$2.4(1) \times 10^{-1}$</td>
<td>$2.05(9) \times 10^{-1}$</td>
<td>$1.81(6) \times 10^{-1}$</td>
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<tr>
<td>C-Pb</td>
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<td></td>
<td>$e^-$</td>
<td>$4.7(1) \times 10^{-1}$</td>
<td>$4.2(1) \times 10^{-1}$</td>
<td>$4.06(7) \times 10^{-1}$</td>
</tr>
<tr>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$9.1(3) \times 10^{-3}$</td>
<td>$9.0(3) \times 10^{-3}$</td>
<td>$8.95(1) \times 10^{-3}$</td>
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<tr>
<td>$P_0(0) = 1$</td>
<td>$e^-$</td>
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<td>$1.353(5) \times 10^{-1}$</td>
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<tr>
<td>C</td>
<td>$\gamma$</td>
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<td>$8.9(1) \times 10^{-3}$</td>
<td>$9.3(3) \times 10^{-3}$</td>
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<td></td>
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<td>$9(3) \times 10^{-5}$</td>
<td>$5(1) \times 10^{-5}$</td>
<td>$7(3) \times 10^{-5}$</td>
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<tr>
<td>N</td>
<td>$\gamma$</td>
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<td>$4(2) \times 10^{-6}$</td>
<td>$3(1) \times 10^{-6}$</td>
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<td></td>
<td>$e^-$</td>
<td>$0(0)$</td>
<td>$0(0)$</td>
<td>$0(0)$</td>
</tr>
<tr>
<td>Fe</td>
<td>$\gamma$</td>
<td>$1.20(4) \times 10^{-1}$</td>
<td>$1.209(4) \times 10^{-1}$</td>
<td>$1.19(1) \times 10^{-1}$</td>
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<td></td>
<td>$e^-$</td>
<td>$1.9(4) \times 10^{-3}$</td>
<td>$1.39(4) \times 10^{-3}$</td>
<td>$1.3(4) \times 10^{-3}$</td>
</tr>
<tr>
<td>Pb</td>
<td>$\gamma$</td>
<td>$2.00(5) \times 10^{-1}$</td>
<td>$1.987(5) \times 10^{-1}$</td>
<td>$1.92(2) \times 10^{-1}$</td>
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<tr>
<td></td>
<td>$e^-$</td>
<td>$1.1(1) \times 10^{-2}$</td>
<td>$9.0(1) \times 10^{-3}$</td>
<td>$8.9(3) \times 10^{-3}$</td>
</tr>
<tr>
<td>C-N</td>
<td>$\gamma$</td>
<td>$3.6(2) \times 10^{-3}$</td>
<td>$3.5(2) \times 10^{-3}$</td>
<td>$3.9(2) \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.9(1) \times 10^{-5}$</td>
<td>$4.1(2) \times 10^{-5}$</td>
<td>$2(1) \times 10^{-5}$</td>
</tr>
<tr>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$5.7(2) \times 10^{-2}$</td>
<td>$6(3) \times 10^{-2}$</td>
<td>$5.9(9) \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$1.02(4) \times 10^{-3}$</td>
<td>$9.3(4) \times 10^{-4}$</td>
<td>$7.8(9) \times 10^{-4}$</td>
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<td>$\gamma$</td>
<td>$1.53(6) \times 10^{-1}$</td>
<td>$1.31(4) \times 10^{-1}$</td>
<td>$1.15(4) \times 10^{-1}$</td>
</tr>
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<td></td>
<td>$e^-$</td>
<td>$8.1(3) \times 10^{-3}$</td>
<td>$6.8(2) \times 10^{-3}$</td>
<td>$7.9(1) \times 10^{-3}$</td>
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<tr>
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<td>$\gamma$</td>
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<td>$6.3(2) \times 10^{-2}$</td>
<td>$6.04(9) \times 10^{-2}$</td>
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<td>$8.7(3) \times 10^{-4}$</td>
<td>$8.9(9) \times 10^{-4}$</td>
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Table 5.6: Mean photon and electron transmittance rates of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.1$ cm single-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 1$ cm single-region slab of pure materials, binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary.

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<th>Transmittance</th>
<th>SMACH</th>
<th>E &lt;sub&gt;e^-&lt;/sub&gt; = 0.1 MeV, L = 0.1 cm</th>
<th>E &lt;sub&gt;\gamma&lt;/sub&gt; = 0.1 MeV, L = 1 cm</th>
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</tr>
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<td>γ</td>
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<td>8.2(3)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>7.5(4)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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<tr>
<td></td>
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<td>0(0)</td>
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<tr>
<td>Fe</td>
<td>γ</td>
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<td>1.6(1)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>1.5(2)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>1(1)×10&lt;sup&gt;-6&lt;/sup&gt;</td>
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</tr>
<tr>
<td>Pb</td>
<td>γ</td>
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<td>2(1)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
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<td>0(0)</td>
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<td>γ</td>
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<td>1.0222(3)×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>9.1(4)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>1.677236(4)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>1.903792(6)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>0(0)</td>
<td></td>
</tr>
<tr>
<td>C-Fe</td>
<td>γ</td>
<td>2.2216(1)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.744(1)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.0(2)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>6.557299(6)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>4.57447(2)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
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<td></td>
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<td>C-Pb</td>
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<td>6.9958(2)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>5(1)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>3.273109(2)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>4.113697(3)×10&lt;sup&gt;-7&lt;/sup&gt;</td>
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<td></td>
</tr>
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<td>γ</td>
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<td>2.4(1)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.4(2)×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>4(1)×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>4.4(9)×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>4(3)×10&lt;sup&gt;-6&lt;/sup&gt;</td>
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<td>γ</td>
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<td>9.963(1)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>9.956(4)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
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</tr>
<tr>
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<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>4.14(7)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>4.25(2)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>4.10(7)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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</tr>
<tr>
<td>N</td>
<td>γ</td>
<td>9.99992(0)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>9.99992(0)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>9.99991(1)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
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<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>3(1)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>3(1)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>3.1(2)×10&lt;sup&gt;-5&lt;/sup&gt;</td>
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<tr>
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<td>γ</td>
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<td>1.0791(4)</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>5.6(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>6.40(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>5.99(9)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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</tr>
<tr>
<td>Pb</td>
<td>γ</td>
<td>9.80(6)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>9.743(6)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>9.46(2)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>5.5(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>5.31(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>5.07(8)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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<td>γ</td>
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<td>9.957(3)×10&lt;sup&gt;-1&lt;/sup&gt;</td>
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<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>2.27(9)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>2.31(9)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>2.30(5)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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</tr>
<tr>
<td>C-Fe</td>
<td>γ</td>
<td>1.034(2)</td>
<td>1.037(2)</td>
<td>1.034(1)</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>6.21(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>6.59(3)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>7.5(1)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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</tr>
<tr>
<td>C-Pb</td>
<td>γ</td>
<td>1.038(2)</td>
<td>1.039(1)</td>
<td>1.0243(6)</td>
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</tr>
<tr>
<td></td>
<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>6.42(7)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>6.56(5)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>8.02(5)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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<tr>
<td>C-Fe</td>
<td>$P_0(0) = 1$</td>
<td>γ</td>
<td>1.041(2)</td>
<td>1.040(2)</td>
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<td>e&lt;sup&gt;-&lt;/sup&gt;</td>
<td>6.28(2)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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<td>7.4(1)×10&lt;sup&gt;-2&lt;/sup&gt;</td>
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Table 5.7: Relative error of mean photon and electron reflectance and transmittance rates of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.1$ cm single-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 1$ cm single-region slab of pure materials, binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary compared against single-scatter and condensed history benchmark results.

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<th>Transmittance</th>
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<tr>
<td>C</td>
<td>$\gamma$</td>
<td>0.01(5)</td>
<td>-0.03(5)</td>
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<td>$e^-$</td>
<td>-0.33(6)</td>
<td>-0.071(8)</td>
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<td>Fe</td>
<td>$\gamma$</td>
<td>-0.08(2)</td>
<td>-0.03(2)</td>
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<td>$e^-$</td>
<td>0.122(3)</td>
<td>0.002(3)</td>
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<td>$\gamma$</td>
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<td>0.01(2)</td>
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<td>$e^-$</td>
<td>0.068(2)</td>
<td>0.025(2)</td>
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<td>$E_{e^-} = 0.1$ MeV, $L = 1$ cm</td>
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<tr>
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<td>$\gamma$</td>
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<td>-0.01(4)</td>
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<td>$\gamma$</td>
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<td>-0.05(3)</td>
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<td>-0.23(3)</td>
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<td>$\gamma$</td>
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<td>-0.13(2)</td>
<td>-0.04(3)</td>
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<td>$\gamma$</td>
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<td>-0.01(3)</td>
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<td>-0.25(3)</td>
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<td>$E_{\gamma} = 10$ MeV, $L = 1$ cm</td>
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<td>$\gamma$</td>
<td>-0.02(3)</td>
<td>0.04(4)</td>
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<td>0.4(6)</td>
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<td>-0.2(4)</td>
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<td>–</td>
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<td>$\gamma$</td>
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<td>0.1(1)</td>
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<td>$\gamma$</td>
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<td>-0.01(5)</td>
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<td>-0.2(1)</td>
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<td>0.0(1)</td>
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Table 5.8: Absolute error of select mean photon and electron reflectance and transmittance rates where the relative error is relatively high because of a small benchmark value on single-region slab problems

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<td>-2(4)×10(^{-5})</td>
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<td>( \gamma )</td>
<td>1(1)×10(^{-6})</td>
<td>1(1)×10(^{-6})</td>
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<td>-2(2)×10(^{-6})</td>
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<td>C-Fe</td>
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<tr>
<td>C-Pb</td>
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<td>1.9958(1)×10(^{-5})</td>
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<tr>
<td></td>
<td>e(^-)</td>
<td>3.273109(2)×10(^{-7})</td>
<td>4.113697(3)×10(^{-7})</td>
<td></td>
</tr>
</tbody>
</table>
Table 5.9: Mean electron material-dependent energy deposition of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.1$ cm single-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 1$ cm single-region slab of pure materials, binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary.

<table>
<thead>
<tr>
<th>Case</th>
<th>Mat</th>
<th>Energy Deposition [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>SS</td>
</tr>
<tr>
<td>$E_{e^-} = 0.1$ MeV, $L = 0.01$ cm</td>
<td>C</td>
<td>9.725(1)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>4.13(1)×10^{-4}</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>7.988(3)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>5.754(4)×10^{-2}</td>
</tr>
<tr>
<td>C-N</td>
<td>C</td>
<td>9.7189(5)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>5.9(5)×10^{-5}</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>2.1(3)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>6.4(2)×10^{-2}</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C</td>
<td>1.9(3)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>4.7(1)×10^{-2}</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C</td>
<td>2.9(3)×10^{-2}</td>
</tr>
<tr>
<td>$P_0(0) = 1$</td>
<td>Fe</td>
<td>5.8(2)×10^{-2}</td>
</tr>
<tr>
<td>$E_{e^-} = 0.1$ MeV, $L = 0.01$ cm</td>
<td>C</td>
<td>1.090(7)×10^{-1}</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>2(1)×10^{-8}</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>1.35(3)</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>3.23(4)</td>
</tr>
<tr>
<td>C-N</td>
<td>C</td>
<td>2.7(2)×10^{-2}</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>1.4(1)×10^{-5}</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>1.72(5)×10^{-1}</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>4.5(3)×10^{-1}</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C</td>
<td>2.4(1)×10^{-1}</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>1.8(1)</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C</td>
<td>1.44(6)×10^{-1}</td>
</tr>
<tr>
<td>$P_0(0) = 1$</td>
<td>Fe</td>
<td>5.6(3)×10^{-1}</td>
</tr>
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</table>
Table 5.10: Relative error of mean electron material-dependent energy deposition of $E_{e^{-}} = 0.1 \text{ MeV}$ electron beam source problems in a $L = 0.1 \text{ cm}$ single-region slab and of $E_{\gamma} = 1 \text{ MeV}$ photon beam source problems in a $L = 1 \text{ cm}$ single-region slab of pure materials, binary Markov mixtures, and a binary Markov mixture of carbon and iron starting with carbon at the boundary compared against single-scatter and condensed history benchmark results.

<table>
<thead>
<tr>
<th>Case</th>
<th>Material</th>
<th>$E_{e^{-}} = 0.1 \text{ MeV}, L = 0.1 \text{ cm}$</th>
<th>$E_{\gamma} = 10 \text{ MeV}, L = 1 \text{ cm}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>CH</td>
</tr>
<tr>
<td>C</td>
<td>C</td>
<td>0.009</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>0.145</td>
<td>0.169</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>0.055</td>
<td>0.018</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>0.064</td>
<td>-0.019</td>
</tr>
<tr>
<td>C-N</td>
<td>C</td>
<td>-0.025</td>
<td>-0.033</td>
</tr>
<tr>
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<td>N</td>
<td>63.824</td>
<td>56.217</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C</td>
<td>-0.107</td>
<td>-0.084</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>0.115</td>
<td>0.065</td>
</tr>
<tr>
<td>C-Pb</td>
<td>C</td>
<td>-0.013</td>
<td>0.041</td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>0.117</td>
<td>0.011</td>
</tr>
<tr>
<td>C-Fe $P_{0}(0) = 1$</td>
<td>C</td>
<td>-0.325</td>
<td>-0.299</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>0.254</td>
<td>0.190</td>
</tr>
</tbody>
</table>

Table 5.11: Mean absolute relative error of mean photon and electron leakage rates and material-dependent electron energy deposition compared against SS and CH benchmark results for single-region slab problems.

<table>
<thead>
<tr>
<th></th>
<th>SS</th>
<th>CH</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle R \rangle_{\gamma}$</td>
<td>0.08(3)</td>
<td>0.05(8)</td>
</tr>
<tr>
<td>$\langle T \rangle_{\gamma}$</td>
<td>0.08(5)</td>
<td>0.05(1)</td>
</tr>
<tr>
<td>$\langle R \rangle_{e^{-}}$</td>
<td>0.175(6)</td>
<td>0.10(4)</td>
</tr>
<tr>
<td>$\langle T \rangle_{e^{-}}$</td>
<td>0.19(6)</td>
<td>0.073(7)</td>
</tr>
<tr>
<td>$E_{e^{-}} \text{ Dep.}$</td>
<td>0.150</td>
<td>0.136</td>
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</table>
Table 5.12: Mean photon and electron reflectance rates of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.01$ cm multi-region slab and of $E_\gamma = 1$ MeV photon beam source problems in a $L = 0.5$ cm multi-region slab comprised of pure material and binary Markov mixed regions with an interface at $x = L/2$

<table>
<thead>
<tr>
<th>Case</th>
<th>Particle</th>
<th>SS</th>
<th>Reflectance</th>
<th>SMACHE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>CH</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>N</td>
<td>$\gamma$</td>
<td>$1.06(3)\times10^{-3}$</td>
<td>$1.06(3)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.46(2)\times10^{-2}$</td>
<td>$3.94(2)\times10^{-2}$</td>
<td>$4.01(3)\times10^{-2}$</td>
</tr>
<tr>
<td>N</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.12(3)\times10^{-3}$</td>
<td>$1.08(3)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.45(2)\times10^{-2}$</td>
<td>$3.91(2)\times10^{-2}$</td>
<td>$3.89(3)\times10^{-2}$</td>
</tr>
<tr>
<td>C</td>
<td>Fe</td>
<td>$\gamma$</td>
<td>$2.02(4)\times10^{-3}$</td>
<td>$2.39(5)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.46(2)\times10^{-2}$</td>
<td>$3.94(2)\times10^{-2}$</td>
<td>$3.66(3)\times10^{-2}$</td>
</tr>
<tr>
<td>Fe</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.16(1)\times10^{-2}$</td>
<td>$1.10(1)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$2.868(5)\times10^{-1}$</td>
<td>$2.515(5)\times10^{-1}$</td>
<td>$2.519(6)\times10^{-1}$</td>
</tr>
<tr>
<td>C</td>
<td>Pb</td>
<td>$\gamma$</td>
<td>$1.91(4)\times10^{-3}$</td>
<td>$1.95(4)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.46(2)\times10^{-2}$</td>
<td>$3.94(2)\times10^{-2}$</td>
<td>$3.66(3)\times10^{-2}$</td>
</tr>
<tr>
<td>Pb</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.07(1)\times10^{-2}$</td>
<td>$7.69(9)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.366(5)\times10^{-1}$</td>
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<td>$5.001(7)\times10^{-1}$</td>
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<tr>
<td>C-Fe</td>
<td>C-Pb</td>
<td>$\gamma$</td>
<td>$8.5(2)\times10^{-3}$</td>
<td>$9.5(2)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$2.4(1)\times10^{-1}$</td>
<td>$2.05(9)\times10^{-1}$</td>
<td>$1.8121(6)\times10^{-1}$</td>
</tr>
<tr>
<td>C-Pb</td>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$9.5(2)\times10^{-3}$</td>
<td>$6.9(1)\times10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$4.6(1)\times10^{-1}$</td>
<td>$4.2(1)\times10^{-1}$</td>
<td>$4.06(7)\times10^{-1}$</td>
</tr>
<tr>
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<td>N</td>
<td>$\gamma$</td>
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<td>$1.64(4)\times10^{-3}$</td>
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<td>$2(1)\times10^{-5}$</td>
<td>$1(1)\times10^{-5}$</td>
</tr>
<tr>
<td>N</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.56(4)\times10^{-3}$</td>
<td>$1.54(4)\times10^{-3}$</td>
</tr>
<tr>
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<td>$e^-$</td>
<td>$5(1)\times10^{-5}$</td>
<td>$5(1)\times10^{-5}$</td>
<td>$4(1)\times10^{-5}$</td>
</tr>
<tr>
<td>C</td>
<td>Fe</td>
<td>$\gamma$</td>
<td>$2.49(2)\times10^{-2}$</td>
<td>$2.41(2)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$7.6(3)\times10^{-4}$</td>
<td>$6.8(3)\times10^{-4}$</td>
<td>$7.2(9)\times10^{-4}$</td>
</tr>
<tr>
<td>Fe</td>
<td>C</td>
<td>$\gamma$</td>
<td>$2.72(2)\times10^{-2}$</td>
<td>$2.58(2)\times10^{-2}$</td>
</tr>
<tr>
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<td>$1.30(4)\times10^{-3}$</td>
<td>$1.15(4)\times10^{-3}$</td>
<td>$1.1(1)\times10^{-3}$</td>
</tr>
<tr>
<td>C</td>
<td>Pb</td>
<td>$\gamma$</td>
<td>$8.9(1)\times10^{-2}$</td>
<td>$8.72(4)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$5.8(3)\times10^{-3}$</td>
<td>$5.52(8)\times10^{-3}$</td>
<td>$5.7(2)\times10^{-3}$</td>
</tr>
<tr>
<td>Pb</td>
<td>C</td>
<td>$\gamma$</td>
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<td>$8.61(4)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$9.1(3)\times10^{-3}$</td>
<td>$8.10(9)\times10^{-3}$</td>
<td>$7.9(3)\times10^{-3}$</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C-Pb</td>
<td>$\gamma$</td>
<td>$5.9(4)\times10^{-2}$</td>
<td>$6.1(4)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
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<td>$2.4(1)\times10^{-3}$</td>
<td>$2.23(5)\times10^{-3}$</td>
</tr>
<tr>
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<td>C-Fe</td>
<td>$\gamma$</td>
<td>$5.4(4)\times10^{-2}$</td>
<td>$5.3(3)\times10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$6.1(4)\times10^{-3}$</td>
<td>$5.8(3)\times10^{-3}$</td>
<td>$6.8(1)\times10^{-3}$</td>
</tr>
</tbody>
</table>
Table 5.13: Mean photon and electron transmittance rates of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.01$ cm multi-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 0.5$ cm multi-region slab comprised of pure material and binary Markov mixed regions with an interface at $x = L/2$

<table>
<thead>
<tr>
<th>Case</th>
<th>Particle</th>
<th>SS</th>
<th>Transmittance</th>
<th>SMACHE</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td>CH</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>N</td>
<td>$\gamma$</td>
<td>$1.77(4)\times 10^{-3}$</td>
<td>$1.85(4)\times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
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<td>$3.475(7)\times 10^{-1}$</td>
</tr>
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<td>C</td>
<td>$\gamma$</td>
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<td>$1.87(4)\times 10^{-3}$</td>
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<td>$3.390(5)\times 10^{-1}$</td>
<td>$3.228(7)\times 10^{-1}$</td>
</tr>
<tr>
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<td>Fe</td>
<td>$\gamma$</td>
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<td>$4(1)\times 10^{-4}$</td>
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<td>$e^-$</td>
<td>$2(1)\times 10^{-6}$</td>
<td>$5(2)\times 10^{-6}$</td>
<td>$0(0)$</td>
</tr>
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<td>Fe</td>
<td>C</td>
<td>$\gamma$</td>
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<td>$1.85(4)\times 10^{-3}$</td>
</tr>
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<td>$0(0)$</td>
<td>$0(0)$</td>
</tr>
<tr>
<td>C</td>
<td>Pb</td>
<td>$\gamma$</td>
<td>$1.0(1)\times 10^{-4}$</td>
<td>$1.2(1)\times 10^{-4}$</td>
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<td>$2(2)\times 10^{-6}$</td>
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<td>C</td>
<td>$\gamma$</td>
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<td>C-Pb</td>
<td>$\gamma$</td>
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<td>$7.0(4)\times 10^{-4}$</td>
</tr>
<tr>
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<td>$e^-$</td>
<td>$2(2)\times 10^{-6}$</td>
<td>$6.6(7)\times 10^{-6}$</td>
<td>$6(3)\times 10^{-6}$</td>
</tr>
<tr>
<td>C-Pb</td>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$1.6(1)\times 10^{-3}$</td>
<td>$2.07(9)\times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$4(3)\times 10^{-6}$</td>
<td>$5.1(1)\times 10^{-6}$</td>
<td>$2(2)\times 10^{-6}$</td>
</tr>
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<td>C</td>
<td>N</td>
<td>$\gamma$</td>
<td>$9.971(1)\times 10^{-1}$</td>
<td>$9.971(1)\times 10^{-1}$</td>
</tr>
<tr>
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<td>$e^-$</td>
<td>$1.28(1)\times 10^{-2}$</td>
<td>$1.29(1)\times 10^{-2}$</td>
<td>$1.25(1)\times 10^{-2}$</td>
</tr>
<tr>
<td>N</td>
<td>C</td>
<td>$\gamma$</td>
<td>$9.972(1)\times 10^{-1}$</td>
<td>$9.972(1)\times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$1.24(1)\times 10^{-2}$</td>
<td>$1.25(1)\times 10^{-2}$</td>
<td>$1.24(1)\times 10^{-2}$</td>
</tr>
<tr>
<td>C</td>
<td>Fe</td>
<td>$\gamma$</td>
<td>$1.0101(2)$</td>
<td>$1.0088(2)$</td>
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<tr>
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<td>$e^-$</td>
<td>$6.06(3)\times 10^{-2}$</td>
<td>$6.29(3)\times 10^{-2}$</td>
<td>$5.98(9)\times 10^{-2}$</td>
</tr>
<tr>
<td>Fe</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.0104(2)$</td>
<td>$1.0092(2)$</td>
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<tr>
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<td>$e^-$</td>
<td>$5.79(3)\times 10^{-2}$</td>
<td>$6.10(3)\times 10^{-2}$</td>
<td>$5.85(8)\times 10^{-2}$</td>
</tr>
<tr>
<td>C</td>
<td>Pb</td>
<td>$\gamma$</td>
<td>$1.054(1)$</td>
<td>$1.0485(4)$</td>
</tr>
<tr>
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<td>$e^-$</td>
<td>$7.8(1)\times 10^{-2}$</td>
<td>$7.53(3)\times 10^{-2}$</td>
<td>$7.1(1)\times 10^{-2}$</td>
</tr>
<tr>
<td>Pb</td>
<td>C</td>
<td>$\gamma$</td>
<td>$1.053(1)$</td>
<td>$1.0500(4)$</td>
</tr>
<tr>
<td></td>
<td>$e^-$</td>
<td>$7.2(1)\times 10^{-2}$</td>
<td>$7.25(3)\times 10^{-2}$</td>
<td>$6.80(9)\times 10^{-2}$</td>
</tr>
<tr>
<td>C-Fe</td>
<td>C-Pb</td>
<td>$\gamma$</td>
<td>$1.026(2)$</td>
<td>$1.025(2)$</td>
</tr>
<tr>
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<td>$e^-$</td>
<td>$7.2(1)\times 10^{-2}$</td>
<td>$7.03(9)\times 10^{-2}$</td>
<td>$8.71(3)\times 10^{-2}$</td>
</tr>
<tr>
<td>C-Pb</td>
<td>C-Fe</td>
<td>$\gamma$</td>
<td>$1.036(3)$</td>
<td>$1.034(3)$</td>
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<tr>
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<td>$e^-$</td>
<td>$6.32(9)\times 10^{-2}$</td>
<td>$6.63(8)\times 10^{-2}$</td>
<td>$7.65(3)\times 10^{-2}$</td>
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Table 5.14: Relative error of mean photon and electron reflectance and transmittance rates of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.01$ cm multi-region slab and of $E_{\gamma} = 1$ MeV photon beam source problems in a $L = 0.5$ cm multi-region slab comprised of pure material and binary Markov mixed regions with an interface at $x = L/2$ compared against single-scatter and condensed history benchmark results.

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<th>Transmittance</th>
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<td>C</td>
<td>$\gamma$</td>
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<td>-0.05(4)</td>
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<td>Fe</td>
<td>$\gamma$</td>
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<td>C</td>
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<td>0.0001(1)</td>
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<td>C-Fe</td>
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<td>C</td>
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<td>-0.1(2)</td>
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<td>Fe</td>
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<td>C</td>
<td>$\gamma$</td>
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<td>0.0(1)</td>
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<td>Pb</td>
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<td>C</td>
<td>$\gamma$</td>
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<td>-0.03(4)</td>
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<td>C-Pb</td>
<td>$\gamma$</td>
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<td>0.07(6)</td>
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<td>C-Fe</td>
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Table 5.15: Absolute error of select mean photon and electron reflectance and transmittance rates where the relative error is relatively on multi-region slab problems

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<td>C-Fe</td>
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<td>C</td>
<td>N</td>
<td>e−</td>
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<td>C-Pb</td>
<td>γ</td>
<td>1.2(4)×10^{-2}</td>
</tr>
<tr>
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<td>C-Pb</td>
<td>C-Fe</td>
<td>γ</td>
<td>1.3(4)×10^{-2}</td>
</tr>
<tr>
<td>(R)</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>e−</td>
<td>Fe</td>
<td>C</td>
<td>e−</td>
<td>2(1)×10^{-6}</td>
</tr>
<tr>
<td></td>
<td>0(0)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pb</td>
<td>C</td>
<td>e−</td>
<td>0.0(3)×10^{-5}</td>
</tr>
<tr>
<td></td>
<td>2(2)×10^{-2}</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>γ</td>
<td>C-Fe</td>
<td>C-Pb</td>
<td>e−</td>
<td>-1.51(4)×10^{-1}</td>
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<tr>
<td></td>
<td>-1.3(1)×10^{-2}</td>
<td></td>
<td></td>
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<tr>
<td>(T)</td>
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<tr>
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<td>C-Fe</td>
<td>e−</td>
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<td>-1.3(1)×10^{-2}</td>
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Table 5.16: Mean electron material-dependent energy deposition of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.01$ cm multi-region slab and of $E_\gamma = 1$ MeV photon beam source problems in a $L = 0.5$ cm multi-region slab comprised of pure material and binary Markov mixed regions with an interface at $x = L/2$.

<table>
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<td>2.62$\times 10^{-5}$</td>
</tr>
<tr>
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<td>Fe</td>
<td>C</td>
<td>8.909(2)$\times 10^{-2}$</td>
<td>8.718(2)$\times 10^{-2}$</td>
</tr>
<tr>
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<td>Fe</td>
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<td>1.088(2)$\times 10^{-2}$</td>
<td>9.947$\times 10^{-3}$</td>
</tr>
<tr>
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<td>6$\times 10^{-7}$</td>
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<td>8.967(2)$\times 10^{-2}$</td>
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<td>7.32$\times 10^{-3}$</td>
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<td>8(2)$\times 10^{-7}$</td>
<td>7$\times 10^{-7}$</td>
</tr>
<tr>
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<td>6.234(4)$\times 10^{-2}$</td>
<td>6.114$\times 10^{-2}$</td>
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<td>Pb</td>
<td>C</td>
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<td>8.967(2)$\times 10^{-2}$</td>
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<td>7$\times 10^{-7}$</td>
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<td>6.234(4)$\times 10^{-2}$</td>
<td>6.114$\times 10^{-2}$</td>
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<td>C-Pb</td>
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<td>2.1(3)$\times 10^{-2}$</td>
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<tr>
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<td>C-Fe</td>
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<td>7.9$\times 10^{-6}$</td>
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<td>1.0(5)$\times 10^{-7}$</td>
<td>3$\times 10^{-8}$</td>
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<tr>
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<td>Fe</td>
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<td>9.2(1)$\times 10^{-3}$</td>
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<td>C-Pb</td>
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<td>7.5(4)$\times 10^{-2}$</td>
<td>7.3(3)$\times 10^{-2}$</td>
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<tr>
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<td>1.02$\times 10^{-1}$</td>
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<td>2.8(3)$\times 10^{-1}$</td>
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<td>1.09$\times 10^{-1}$</td>
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<td>2.2(2)$\times 10^{-1}$</td>
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Table 5.17: Relative error of mean electron material-dependent energy deposition of $E_{e^-} = 0.1$ MeV electron beam source problems in a $L = 0.01$ cm multi-region slab and of $E_\gamma = 1$ MeV photon beam source problems in a $L = 0.5$ cm multi-region slab comprised of pure material and binary Markov mixed regions with an interface at $x = L/2$ compared against single-scatter and condensed history benchmark results.

<table>
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<th>$E_{\gamma} = 10$ MeV, $L = 0.5$ cm</th>
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<td>0.191</td>
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<td>Fe</td>
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<td>0.006</td>
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<td>Pb</td>
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<td>-0.7</td>
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<td>-0.53</td>
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Table 5.18: Absolute error of select material-dependent electron energy deposition where the relative error is relatively high on multi-region slab problems.

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<th>Absolute Error</th>
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<td>N</td>
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<tr>
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<td>Fe</td>
<td>C</td>
<td>C</td>
</tr>
<tr>
<td></td>
<td>C-Fe</td>
<td>C-Pb</td>
<td>Pb</td>
</tr>
<tr>
<td></td>
<td>C-Pb</td>
<td>C-Fe</td>
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<td>$\gamma$</td>
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<td>C</td>
</tr>
<tr>
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<td>C-Pb</td>
<td>C-Fe</td>
<td>Fe</td>
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Table 5.19: Mean absolute relative error of mean photon and electron leakage rates and material-dependent electron energy deposition compared against SS and CH benchmark results for multi-region slab problems

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<th>CH</th>
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<tr>
<td>$\langle R \rangle_\gamma$</td>
<td>0.113(9)</td>
<td>0.06(1)</td>
</tr>
<tr>
<td>$\langle T \rangle_\gamma$</td>
<td>0.088(9)</td>
<td>0.05(2)</td>
</tr>
<tr>
<td>$\langle R \rangle_{e^-}$</td>
<td>0.16(3)</td>
<td>0.11(4)</td>
</tr>
<tr>
<td>$\langle T \rangle_{e^-}$</td>
<td>0.4(2)</td>
<td>0.19(4)</td>
</tr>
<tr>
<td>$E_{e^-}$ Dep.</td>
<td>0.275</td>
<td>0.301</td>
</tr>
</tbody>
</table>
CHAPTER 6

Conclusions and Future Work

6.1 Conclusions

Understanding the characteristics of a photon-electron field is important for a number of applications, in which materials may heat up or be damaged from deposited energy. This includes, but is not limited to, inertial confinement fusion problems, radiotherapy treatment, power production in pebble bed reactors, and light propagation. One way of modeling a photon-electron field is by using a Monte Carlo approach in which the trajectories of photons and electrons are randomly simulated. However, an electron may experience an order of $10^5$ interactions within the span of a few millimeters, and conducting a detailed simulation is often computationally expensive for routine calculations.

The condensed history method is a well-known and widely-used computational technique that has been developed to improve runtime by segmenting an electron history into steps comprised of numerous electron interactions. This method relies on multi-scatter probability distributions that assume a homogeneous background material and breaks down for problems in which the material properties have random spatial variation given by material mixing probabilities. Methods have been developed to model transport in these stochastic material mixtures, but most of this work applies to neutral particle transport with minimal literature addressing the challenges of electron transport in stochastic media. Limited work has been done in applying electron transport methods to stochastic media problems, and to
model electron transport in stochastic mixtures with current methods, the computationally expensive “brute force” approach of simulating each individual interaction is required.

The focus of this dissertation topic was to develop a statistical condensed history model and simulation method that sufficiently accounts for the underlying randomness of material properties given some prescribed distribution function; specifically, extending computational capabilities of the Class I condensed history algorithms to binary, Markovian-mixed media, which involved deriving multi-scatter distributions applicable to substep and step lengths that cross many material boundaries. The angular deflection and energy loss straggling multi-scatter distributions for a single binary Markovian-mixed realization are derived in Chapter 4 following a similar analysis as Goudsmit and Sauderson, Blunck and Leisegang, Chechin and Ermilova, and Seltzer as discussed in Chapter 3. A transit-length distribution is also derived in Chapter 4 to preserve the mean and compute the ensemble average distributions for all possible binary, Markovian-mixed material realization combinations that an electron may traverse within a length. The transit-length distribution is also used to compute the ensemble average mean free paths of secondary particle production, which were used to sample secondary particles in an analog manner. Additionally, this work presents a new capability of computing material-dependent electron energy deposition that current condensed history algorithms can not easily execute.

The derived ensemble average angular deflection and energy loss straggling multi-scatter distributions and mean free paths were verified in Chapter 5. This verification was conducted by generating several full binary Markovian-mixed material realizations and computing the corresponding multi-scatter distribution and mean free path for each realization. The benchmark results were computed by taking the average of these multi-scatter distributions and mean free paths and comparing them against the ensemble average angular deflection and energy loss straggling multi-scatter distributions and mean free paths that are derived in Chapter 4 using the transit-length distribution. This comparison showed that the ensemble average angular deflection and energy loss straggling multi-scatter distributions as well as
mean free paths computed using the transit-length distribution agree within statistical un-
certainty of the respective benchmark ensemble average angular deflection and energy loss
multi-scatter straggling distributions and mean free paths.

Validation of a condensed history algorithm for stochastic media, called SMACHE, using
the ensemble average angular deflection and energy loss straggling multi-scatter distribu-
tions and mean free paths derived in Chapter 4 was conducted by comparing mean photon
and electron leakage rates as well as material-dependent electron energy deposition results
against benchmark results generated using a single-scatter and condensed history approach
with MCNP6 on fully generated binary Markovian-mixed realizations. Different combina-
tions of carbon, nitrogen (air), iron, and lead were investigated to demonstrate the accuracy
of SMACHE for different $Z$ materials on $E_{e^-} = 0.1$ MeV electron beam source and $E_\gamma = 10$
MeV photon beam source problems on an infinite slab of a pure background material and a
binary, Markovian-mixed background material with and without an internal interface.

The results demonstrate SMACHE’s capabilities in computing mean particle leakage rates
and material-dependent electron energy deposition results for single-region and multi-region
slab geometries. For single-region problems, SMACHE achieved a mean absolute relative
error of about 5% for photon leakage rates, and about 10% for electron leakage rates, re-
spectively, compared to CH benchmarks. Compared to SS benchmarks, SMACHE achieved
a mean absolute relative error of about 8% for photon leakage rates, and about 19% for
electron leakage rates, respectively. Notably, this work also demonstrates a new capability
of accurately quantifying material-dependent electron energy deposition results using a con-
densed history approach without the need to generate full material realizations. However,
SMACHE overestimated the electron energy deposition in nitrogen (air) in a carbon-nitrogen
mixture. Not including the carbon-nitrogen case for a single-region, SMACHE achieved a
mean absolute relative error of 15.0% and 0.13.6% for material-dependent electron energy
deposition when compared against SS and CH benchmark results, respectively.

For multi-region problems investigated, SMACHE performed best on particle leakage
rates when compared to CH benchmark results than when compared to SS benchmark results. When compared against CH benchmark results, SMACHE achieved a mean absolute relative error of 6% and 5% for photon reflectance and transmittance rates, respectively, and 11% and 19% for electron reflectance and transmittance rates, respectively. When compared against SS benchmark results, SMACHE achieved a mean absolute relative error of 11.3% and 8.8% for photon reflectance and transmittance rates respectively, and 16% and 40% for electron reflectance and transmittance rates, respectively. The SMACHE achieved a mean absolute relative error of 27.5% and 30.1% for material-dependent electron energy deposition when compared against SS and CH benchmark results, respectively, which is roughly double the mean absolute relative error of the material-dependent electron energy deposition of SMACHE for single-region slab problems. This increase in error is a result of substep truncations that occur at the internal slab interface.

6.2 Future Work

This dissertation presented a method that shows promise for the development of a robust condensed history method that can accurately model photon-electron transport in stochastic media while accelerating computing time by bypassing the need to use a brute-force single-scatter approach on several fully generated material realizations. This dissertation investigated beam source problems on slab geometries for binary, Markovian-mixed media, and future work could be in expanding this repertoire of investigated problems using this method.

Currently, the accuracy of the method investigated in this dissertation is limited by using knowledge of only the preserved material probability of an electron at the beginning of a substep to sample angular deflection, energy loss straggling, and secondary particle production. The number of possible material realizations the electron could have traversed within a substep is reduced if the preserved material probabilities at both the beginning and end of the substep are known. Therefore, deriving a transit-length distribution that accounts for
these two characteristics could further refine the accuracy of sampling the angular deflection, energy loss, and secondary particle production of an electron transporting through a random mixture. Furthermore, the error in material-dependent electron energy deposition noticeably increased on multi-region slab problems. This is a result of the approximations introduced into the solution from substep truncation. Future work could be in improving internal interface crossings.

The accuracy of the photon transport component of SMACHE and the computation of photon leakage rates could be further improved by using a method generally more accurate than the AM approximation. Some methods that could be used instead are CLS, LRP, or CoPS for binary, Markovian-mixed media. Improving the accuracy of the photon transport portion of this code could also lead to improved accuracy in secondary electron generation.

The new method requires that all ensemble average multi-scatter distributions are pre-computed and tabulated, which is currently an inefficient step in SMACHE. Further work could be in investigating ways to reduce this computing time by either improving this computation time or applying a sampling technique such that the ensemble-average multi-scatter distributions do not have to be fully computed before the time of particle simulation and, rather, be sampled from during particle simulation.

The focus of this work was in deriving distributions and quantities that preserve the mean effects of the stochastic background material on the electron as it streams through the background material. Future work can be in developing a methodology to compute higher-order moments using SMACHE.

An ideal condensed history method for stochastic mixtures would be generalized to $N$-ary media as well as other types of stochastic mixtures beyond Markov mixtures. Future work may be in deriving ensemble average multi-scatter distributions for $N$-ary, Markovian-mixed media using a transit-length distribution that is generalized to $N$-ary materials as well as deriving a transit-length distribution for other types of material mixing.
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