Electron Photon Calculations using MCNP

by

David P. Gierga
B.S., Nuclear Engineering (1996)
Rensselaer Polytechnic Institute

Submitted to the Department of Nuclear Engineering in Partial Fulfillment of the Requirements for the Degree of
Master of Science
at the
Massachusetts Institute of Technology
February 1998

© Massachusetts Institute of Technology, 1998. All Rights Reserved.

Author............................................................
Department of Nuclear Engineering
January 16, 1998

Certified by ....................................................... Jacquelyn C. Yanch
Associate Professor of Nuclear Engineering and Whitaker College
Thesis Co-Supervisor

Certified by ........................................................

Kenneth J. Adams
Technical Staff Member, Los Alamos National Laboratory
Thesis Co-Supervisor

Accepted by ....................................................... Lawrence M. Lidsky
Professor of Nuclear Engineering
Chairman, Department Committee on Graduate Students

Science
Electron Photon Calculations using MCNP

by

David P. Gierga

Submitted to the Department of Nuclear Engineering on January 16, 1998, in Partial Fulfillment of the Requirements for the Degree of Master of Science in Nuclear Engineering

ABSTRACT

MCNP4B™ was released in February 1997 with significant enhancements to electron/photon transport methods. As part of this thesis, these enhancements have been verified against a wide range of published electron/photon experiments, spanning high energy bremsstrahlung production to electron transmission and reflection. The impact of several MCNP tally options and physics parameters was explored in detail. The agreement between experiment and simulation was usually within two standard deviations of the experimental and calculational errors. Furthermore, sub-step artifacts for bremsstrahlung production were shown to be mitigated. A detailed suite of electron depth dose calculations in water is also presented. Areas for future code development have also been explored and include the dependence of cell and detector tallies on different bremsstrahlung angular models and alternative variance reduction splitting schemes for bremsstrahlung production.

In addition to the verification study, a Macro Monte Carlo (MMC) algorithm has been developed and implemented into MCNP4B. This algorithm makes use of a previously generated electron data library to perform the electron transport. For this study, MCNP was used to generate the libraries, and the necessary transport information needed in the library for accurate simulations has been determined. The MMC algorithm has been shown to improve the speed of the MCNP calculation by a factor of 1.5-2.25 for a limited range of one-dimensional depth dose in water calculations. The MMC and MCNP calculations show excellent agreement for a range of energies. The agreement between the MMC and MCNP calculation decreases with the incident energy of the electron.

Thesis Co-Advisor: Jacquelyn C. Yanch
Title: Associate Professor of Nuclear Engineering and Whitaker College

Thesis Co-Advisor: Kenneth J. Adams
Title: Technical Staff Member, Los Alamos National Laboratory

™MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory
Acknowledgments

I would like to especially thank Ken Adams for all of his guidance, insight, and patience throughout this project. I would also like to thank everyone else at Los Alamos National Laboratory for their support and encouragement in this work. Professor Yanch deserves thanks as well for her support, and for allowing me to do much of this work off-campus.

I would also like to thank Clint Ballinger for fueling my interest in electron transport, for arranging for me to work at Los Alamos, and for his encouragement throughout this project.

Finally, I owe a great debt of gratitude to my parents for everything that they have done for me over the course of my life.
# Table of Contents

1. Introduction.................................................................................................................. 9
2. Photon Transport in MCNP .......................................................................................... 11
   2.1 Photon Tracks........................................................................................................... 11
   2.2 Thomson Scattering ................................................................................................. 12
   2.3 Photoelectric Effect ................................................................................................. 13
   2.4 Compton Scattering ................................................................................................. 13
   2.5 Pair Production ....................................................................................................... 14
3. Electron Transport in MCNP ....................................................................................... 15
   3.1 Electron Major-steps and Sub-steps .................................................................. 15
   3.2 Condensed History Flow ......................................................................................... 16
   3.3 Collisional Stopping Power .................................................................................... 17
   3.4 Bremsstrahlung ...................................................................................................... 18
   3.5 Energy Straggling .................................................................................................. 18
   3.6 Knock-On Electrons ............................................................................................... 19
4. Bremsstrahlung Verification Calculations ..................................................................... 20
   4.1 Faddegon et al. Experiment .................................................................................. 20
   4.2 O’Dell et al. Experiment ....................................................................................... 29
   4.3 Starfelt and Koch Experiment .............................................................................. 32
5. Electron Transmission and Backscatter ....................................................................... 35
   5.1 Ebert et al. Experiment ......................................................................................... 35
6. Physics Parameter Studies ............................................................................................. 39
   6.1 Bremsstrahlung Angular Models .......................................................................... 39
   6.2 Coherent Scatter .................................................................................................... 43
   6.3 Electron Sub-step size ............................................................................................ 44
   6.4 Energy Grid Sampling ............................................................................................ 47
   6.5 Splitting Schemes for Bremsstrahlung Production .............................................. 54
   6.6 20 MeV Electrons in Water .................................................................................. 63
7. Electron Transport Using Macro Monte Carlo ........................................................... 83
   7.1 Electron Data Library Generation ......................................................................... 83
   7.2 Description of the Macro Monte Carlo Algorithm .............................................. 91
   7.3 MMC Results ......................................................................................................... 95
8. Conclusions .................................................................................................................. 104
9. References .................................................................................................................... 106
Appendix A. MCNP Verification Input Files ................................................................. 110
Appendix B. Modified BNUM Sampling Patch ............................................................. 123
Appendix C. Local Calculation Input File for MMC Library ........................................ 124
Appendix D. Surface Source Formatting Code ............................................................... 125
Appendix E. Post-Processor Library Generation Code ................................................. 126
Appendix F. MMC Energy Grid ...................................................................................... 135
Appendix G. MMC Patch to MCNP .............................................................................. 137
Appendix H. Sample input file for MMC comparisons to MCNP ................................. 144
1. Introduction

The Monte Carlo method is often used to perform radiation transport calculations. Several computer codes are available which can adequately solve the transport equation. One of the most widely used codes is MCNP (Monte Carlo N-Particle). MCNP can perform coupled neutron-photon-electron transport calculations. Chapters 2 and 3 of this thesis outline photon and electron transport as implemented in MCNP. The results of an extensive set of electron photon MCNP verification calculations are presented in Chapters 4-6. Chapter 7 describes an alternative method that was developed for electron transport problems in MCNP.

MCNP4B was released in February 1997 with significant enhancements to electron/photon transport methods\(^1\). These enhancements have been verified against a wide range of published electron/photon experiments, spanning high energy bremsstrahlung production to electron transmission and reflection. These are covered in Chapters 4 through 6. Three sets of bremsstrahlung experiments were simulated. The first verification calculations for bremsstrahlung production used the experimental results of Faddegon\(^2\)\(^-\)\(^4\) for 15 MeV electrons incident on lead, aluminum, and beryllium targets. The calculated integrated bremsstrahlung yields, the bremsstrahlung energy spectra, and the mean energy of the bremsstrahlung beam were compared with experiment. The impact of several MCNP tally options and physics parameters was explored in detail. The second was the experiment of O’Dell\(^5\) which measured the bremsstrahlung spectra from 10 and 20.9 MeV electrons incident on a gold/tungsten target. The final set was a comparison of relative experimental spectra with calculated results for 9.66 MeV electrons incident on tungsten based on the experiment of Starfelt and Koch\(^6\). The transmission experiments of Ebert\(^7\) were also studied, including comparisons of transmission coefficients for 10.2 MeV electrons incident on carbon, silver, and uranium foils. Backscatter coefficients for electrons of a range of energies were also compared. The agreement between experiment and simulation was usually within two standard deviations of the experimental and calculational errors. Furthermore, sub-step artifacts for bremsstrahlung production were shown to be mitigated. A detailed suite of electron depth dose calculations in water is also presented. Areas for future code development have also been explored and include the dependence of cell and detector tallies on different bremsstrahlung angular models and alternative variance reduction splitting schemes for bremsstrahlung production.

In addition to these verification calculations, a new algorithm for electron transport calculations, termed Macro Monte Carlo, was developed and implemented in MCNP. Macro Monte Carlo (MMC) is a Monte Carlo transport method which is designed to utilize a suite of detailed local calculations to perform global calculations. It has primarily been used to help speed up electron calculations with little sacrifice in accuracy\(^8\)\(^-\)\(^11\). We have explored implementing a particular version of MMC in MCNP. This involved library generation of global transport parameters and transport methods to use these parameters. The level of accuracy for various MMC approximations has been studied for energy deposition in a water phantom. The type of electron data library and transport algorithm needed for efficient and accurate results has been defined. The final method has achieved reasonable agreement with standard MCNP calculations, and shown an improvement in calculational efficiency by nearly a factor of two. MCNP uses the condensed history method for electron transport\(^1\); the increase in calculational speed demonstrated for MMC is much greater when compared to single event electron codes rather than condensed history codes.

The essential idea in MMC is to define a volume of physical space, termed a “kugel,” transport particles, using either condensed history or single event Monte Carlo, through this volume, and
tally the particles exiting the volume. This process, performed over many incident energies, can be viewed as a series of local calculations. These tallies are then post-processed to construct a library; the library provides the global information. This library is then used in a new algorithm to transport the particles in a global sense, where the electrons take large-scale, macroscopic kugel steps through the material. The computational acceleration results from the fact that within the kugel there are many interactions which are essentially averaged to produce a net effect, not unlike the condensed history algorithm. Thus, one macro kugel step is equivalent to many electron steps.

As this project developed, several modifications were made to the electron data library to reduce the level of approximation. The data library and transport algorithm differ from previous work in this area\textsuperscript{8-11}. This thesis traces the development of the library, and gives results that provide insight into the various approximations that were made. The development of the transport algorithm is also described.
2. Photon Transport in MCNP

This chapter will describe the implementation of photon physics in MCNP. For a more rigorous description, see Reference 1. The detailed physics package in MCNP will be described since it was used in all of the calculations included in this thesis. The detailed photon physics model in MCNP describes the three major photon interactions: photoelectric effect, Compton (incoherent) scattering, and pair production. Furthermore, Thomson (coherent) scattering and fluorescent photons emitted after photoelectric absorption are included. A simple physics model can also be used, which ignores these last two processes. MCNP can model the secondary electrons generated via photon interactions in three different ways. In any default coupled electron photon calculation (mode p e), any secondary electrons are explicitly transported. This mode of transport was used for all of the verification calculations presented in this thesis. For photon only transport problems (mode p), the thick target bremsstrahlung model may be used in which the electrons are generated but immediately terminated. This eliminates the computationally intensive electron transport. Bremsstrahlung photons produced by these “non-transported” electrons are banked for subsequent transport. This method is the default in MCNP but should be used judiciously. The third option, recommended for mode p problems, is to set the IDES entry on the PHYS:P card to 1, which turns off all electron production, with all secondary electron energy assumed to be deposited locally. This method is acceptable as long as bremsstrahlung generation is not important.

2.1 Photon Tracks

Before describing the individual photon interactions, the basic Monte Carlo methodology for tracking the history for a photon will be explained. One of the fundamental quantities necessary for tracking a particle’s history is the distance to collision. The distance to collision, or path length, is related to the macroscopic cross section, \( \Sigma_t \), of the medium in which the particle history takes place. For photons, \( \Sigma_t \) is usually replaced with \( \mu \), the linear attenuation coefficient. The meaning of the two parameters is identical; both are the probability per unit length that an interaction will take place. The cross section is determined based on the particle’s energy and the material of interest. The probability of a particle traveling a certain distance \( l \) before collision is

\[
p(l) = e^{-\Sigma_t l}
\]

(2.1)

The probability of a particle undergoing a collision between \( l \) and \( l + dl \) is therefore

\[
p(l)dl = e^{-\Sigma_t l} \Sigma_t dl.
\]

(2.2)

If Eq. 2.2 is integrated over the path length of the particle and set equal to some random number \( \xi \), the result is

\[
\xi = \int_0^l e^{-\Sigma_t s} \Sigma_t ds = 1 - e^{-\Sigma_t l}.
\]

(2.3)

Solving for \( l \) gives
The random numbers $\xi$ are evenly distributed between 0 and 1. It follows that $1 - \xi$ follows the same distribution. Thus, the distance to collision is randomly sampled according to

$$l = -\frac{1}{\Sigma} \ln (1 - \xi). \quad (2.4)$$

If no boundary crossings occur, and energy cutoffs are neglected, the distance to collision will equal the particle track length. MCNP also must calculate the distance to boundary surface intercept, to determine if a boundary crossing will take place. If the distance to collision is less than the distance to surface crossing, then the particle will undergo a collision. If the distance to collision exceeds the distance to surface crossing, then a boundary is crossed, and the history continues at the point of boundary crossing. If the distance to collision happens to exactly equal the distance to surface crossing, then the particle is treated as crossing the surface and is started in the next cell. The type of collision is determined by sampling from the various probability distributions described in the next sections. The probability of a photoelectric event, for example, is given by the ratio of the photoelectric cross section to the total cross section at the given photon energy. A discrete probability distribution can be created from the probabilities of each possible interaction. This distribution is then randomly sampled to determine the collision type.

### 2.2 Thomson Scattering

In Thomson, or coherent, scattering, an electron oscillates classically as a response to the electromagnetic field of a passing photon. Over the energy range that Thomson scattering is important, the incident photon has a low enough energy that the electron must be modeled as bound. The oscillating electron then emits photons of the same frequency as the incident radiation. The net effect is the redirection of incident photons with no energy transfer to the medium. Since Thomson scattering involves no energy loss, it is different from all other photon interactions included in MCNP in that no secondary electrons are produced.

The Thomson cross section is of the form

$$T(\mu) = \pi r_0^2 (1 + \mu^2) \quad (2.6)$$

where $r_0$ is the classical electron radius and $\mu = \cos \theta$. The actual cross section is modified by a form factor. The cross section is fairly isotropic at low energies. At high energies, the cross section becomes very forward peaked. This is accounted for by multiplying the standard Thomson cross section (Eq. 2.6) by a form factor that decreases the Thomson cross section for high energies and backward scattering. For high incident photon energies, Thomson scattering is usually ignored because it is very forward peaked.

Since, at high energies, the cross section is forward peaked with no energy loss, it is as if no scattering took place. If a point detector tally is to sample coherent scattering, the point must be on the original particle track, which usually does not occur. Thus, including coherent scatter in...
the simulation can lead to larger detector tally variances. Although coherent scatter is included by
default in the detailed physics photon transport in MCNP, it can be turned off by setting the
NOCOH entry of the PHYS:P card in the input file to 1. The impact of photon physics models on
tallies is investigated further in this thesis. Comparisons of detector tallies to cell tallies are also
done.

2.3 Photoelectric Effect

In the photoelectric effect, an incident photon of energy $E$ interacts with an atom such that
the photon is absorbed, and an orbital electron is emitted. The photoelectron will have kinetic
energy of $E-e$, where $e$ is the binding energy of the electron. The resulting electron vacancy ultimately results in the emission of a combination of characteristic x-rays (fluorescent photons) or Auger electrons. The cross section for the photoelectric effect varies roughly as $Z^4/E^3$, where $Z$ is the atomic number of the material in question.

The shell structure of the atom determines the subsequent radiations that may be emitted following a photoelectric event. The fluorescent yield, defined as the number of characteristic x-rays emitted per shell vacancy, increases with $Z$. The energy of the fluorescent photons determines whether they will be subsequently tracked in the MCNP simulation. The low energy cutoff for photon transport is 1 keV. All fluorescent photons are modeled as being emitted isotropically.

2.4 Compton Scattering

In Compton scattering, an incident photon undergoes a collision with an electron, usually assumed to be free and at rest (see Figure 2.1). As a result of the collision, the photon is scattered with a new energy $E'$, and the electron recoils at an angle $\phi$ with kinetic energy $E - E'$. The scattered photon energy is given by

$$ E' = \frac{E}{1 + \frac{E}{mc^2}(1 - \mu)} $$

where $m$ is the electron mass and $c$ is the speed of light, and $\mu = \cos \theta$. Equation 2.7 describes the energetics of Compton scattering. The probability of such a scattering taking place is described by the Klein-Nishina cross section, $K(E, \mu)$, modified by a form factor. The Klein-Nishina cross section, as implemented in MCNP, is given by

$$ K(\alpha, \mu) \, d\mu = \pi r_0^2 \left( \frac{\alpha'}{\alpha} \right)^2 \left[ \frac{\alpha'}{\alpha} + \frac{\alpha}{\alpha'} + \mu^2 - 1 \right] \, d\mu $$

where $r_0$ is the classical electron radius, and $\alpha$ and $\alpha'$ are the incident and final photon energies given by

$$ \alpha = \frac{E}{mc^2} $$
As described in Ref. 1, the Klein-Nishina cross section is sampled using Kahn's method\textsuperscript{12} for photon energies less than 1.5 MeV, while Koblinger's method\textsuperscript{13,14} is used for energies greater than 1.5 MeV.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{compton_scattering}
\caption{Compton Scattering}
\end{figure}

\textbf{2.5 Pair Production}

Pair production occurs when a photon interacts in the coulomb field of a nucleus and results in the production of an electron positron pair. This process can only take place near a nucleus to conserve energy and momentum. Pair production has a threshold of twice the electron rest mass, or 1.022 MeV. The probability of a pair production for photon energies greater than the threshold rises sharply with energy, and varies approximately as $Z^2$. For coupled electron photon problems in MCNP, the electron and positron pair is banked for subsequent transport, and the photon track is ended. The resulting positron will most likely slow down in the medium, attract an electron, and annihilate. Two photons, each of 0.511 MeV, are produced.
3. Electron Transport in MCNP

Electron transport is necessarily different from either photon or neutron transport. Uncharged particles, such as neutrons or photons, undergo a relatively small number of “catastrophic” collisions as they interact with matter. For photons, these interactions have been previously described, and include the photoelectric effect, Compton scatter, and pair production. Electrons are charged and thus interact continuously through long-range Coulomb forces. An electron typically undergoes roughly $10^4$ more collisions for the same energy loss than a neutral particle. For example, an electron slowing down from 0.5 MeV to 0.0625 MeV will undergo on the order of $10^5$ collisions. A photon need only undergo about 20-30 Compton scatters to reduce its energy from several MeV to 50 keV\(^1\).

Modeling every electron interaction (analog transport) in a Monte Carlo code is not a viable means of simulating the transport of electrons. Non-trivial problems could not be solved without an enormous investment in computer time. One alternative to analog transport is to follow the electrons over path length (or energy loss) increments that account for the combined effect of multiple collisions, without explicitly modeling every interaction. Several multiple-scattering theories have been put forth and attempt to describe the energy loss and angular deflections for electrons. MCNP primarily uses the Bethe-Bloch\(^{40,41}\) model for energy losses, the Goudsmit-Saunderson\(^{15}\) theory for angular deflections, the Landau\(^{16}\) theory of energy straggling, and the Blunck-Leisegang\(^{17}\) additions to Landau theory.

The condensed history algorithm is used in MCNP to transport electrons. In condensed history, multiple scattering theories are applied to a series of steps that combine to equal the electron’s complete history. The steps must be chosen such that they are long enough to include enough collisions for the multiple scattering theories to be satisfied, but short enough so the energy loss is small compared to the kinetic energy of the electron\(^1\). The multiple scattering distributions are sampled at each step in order to describe the change in the energy and direction of the electron. The seminal reference for the condensed history method is Martin J. Berger’s 1963 paper\(^18\). Subsequently, Berger and Seltzer developed the ETRAN\(^{19}\) series of electron-photon transport codes. The Integrated TIGER Series (ITS)\(^{20}\), a set of general electron-photon transport codes, were formulated using ETRAN as a basis. The electron physics in MCNP mirrors the physics in ITS very closely. See Reference 1 for a more detailed description of electron transport in MCNP.

3.1 Electron Major-steps and Sub-steps

The electron history is divided into major steps (also called energy steps), which are in turn divided into smaller substeps. The path length for a major step is $s = s_n - s_{n-1}$. The continuous slowing down approximation (CSDA) relates, on average, the energy and path length such that

$$E_{n-1} - E_n = -\int_{s_{n-1}}^{s_n} \frac{dE}{ds} ds$$

(3.1)
where \(-dE/ds\) is the total stopping power for the appropriate energy and material of interest. MCNP divides the energy loss for each step according to

\[
\frac{E_n}{E_{n-1}} = k
\]

for a constant \(k\). In MCNP, \(k = 2^{-1/8}\), which gives an average loss per step of 8.3%.

Each major step (path length \(s\)) is divided into \(m\) smaller substeps (path length \(s/m\)). An energy grid based on Eq. 3.2 contains all the necessary data for electron transport. At every energy step, the energy straggling theories of Landau and Blunck-Leisegang are exercised. The angular deflections, however, are applied more frequently throughout the electron history, i.e. at every substep. The Goudsmit-Saunderson multiple scattering theory is valid for arbitrary angular deflections, but greater accuracy can be attained by directing the angular deflections to be small and therefore sampling the angle distributions more than once per energy step. Secondary particle production and angular deflections are also sampled every substep, rather than major step. The parameter \(m\), which sets the scale of the substep, is a material dependent parameter, based on the average atomic number \(Z\). Suitable values for \(m\) have been empirically determined, ranging from \(m=2\) for \(Z<6\) to \(m=15\) for \(Z>91\).

Although default values of \(m\) are set in the code, MCNP allows the user to increase this parameter. Very thin material regions may not allow enough electron substeps to adequately follow the electron track. The MCNP manual recommends that electrons should take at least ten substeps in any material of importance. This recommendation is rather conservative, since accurate results have been obtained in some cases with tally bins, or the material itself, only a few substeps thick. The user can vary \(m\) by using the ESTEP option on the appropriate material card in the MCNP input file. Print Table 85 in the MCNP output provides information relevant to electron transport, including DRANGE, which is the size of a major step, in units of g/cm². Consequently, DRANGE/(mp) is the length of a substep in cm.

### 3.2 Condensed History Flow

Parameters necessary in a description of the electron history include the electron energy grid, stopping powers, ranges, energy step sizes, substep sizes, and probability distributions for angular deflections and secondary particle generation. MCNP determines these parameters by precalculation, or by reading in from the electron data file. The collisional energy loss rate is sampled at the beginning of the major step. For this part of the transport, MCNP treats electron energy loss based only on non-radiative processes. Bremsstrahlung is sampled separately, as described in Section 3.4. Only the energy loss rate and straggling parameters are sampled according to the major step; all other transport parameters are sampled during each substep. An energy for the electron at the end of its substep, barring additional loss from secondary processes, is calculated using the present value of the collisional stopping power. Secondary processes, such as electron induced fluorescent x-rays, "knock-on" electrons from electron impact ionization, and bremsstrahlung radiation are then appropriately sampled. The direction of the electron is updated at the end of each substep by sampling the Goudsmit-Saunderson distributions for angular deflection. The maximum number of substeps in the current major step is \(m\). Fewer substeps may be taken if the electron undergoes boundary crossing, or the energy becomes less than the lower energy boundary for that major step. A new major step is begun once either \(m\) substeps have been
taken or a boundary is violated. Then, the process continues, and a new energy loss rate is sampled.

It is important to note that the length of the substep is dependent on the total energy loss rate (see Eq. 3.1), but the projected energy loss for the substep is based on the collisional stopping power. This difference can be justified because when a bremsstrahlung photon is generated, its energy is subtracted from the projected energy loss for the substep, which is based on the collisional stopping power. Electron energy loss to bremsstrahlung is therefore treated directly.

3.3 Collisional Stopping Power

Electrons can lose energy in collisions with atomic electrons, leading to excitation and ionization of the medium. At low electron energies, radiative losses are negligible. The relative importance of ionization to excitation increases rapidly with the energy of the electron. For kinetic energies greater than 150 eV, 95% of the energy loss results in ionization. In water, for example, it takes an average of about 22 eV to ionize an electron, so an abundance of low-energy electrons will be created \(^{39}\). These electrons will be of very low energy, so they will not be followed in MCNP, since the default low energy cutoff is 1 keV. As the electron energy increases, bremsstrahlung becomes important, as discussed in Section 3.4.

The collisional energy loss for electrons in MCNP is based on the restricted stopping power given by Berger \(^{18}\), which gives the energy loss per unit length that results in energy transfers (relative to the kinetic energy \(E\) of the electron) \(E\) less than some maximum \(\varepsilon_{m}\). For electron collisions, quantum mechanics dictates that it is impossible to distinguish between the two outgoing electrons, and the electron with the higher energy is taken by convention to be the primary electron. For these reasons, the parameter \(\varepsilon_{m}\) is set to 0.5, and the restricted stopping power becomes a total stopping power. Berger’s stopping power, in units of MeV-barns, then takes the form

\[
\left(\frac{dE}{ds}\right) = \frac{10^{24} \alpha^2 \hbar^2 c^2 Z}{2 \pi m c^2 \beta^2} \left\{ \log[\tau^2(\tau + 2)] - C_2 + C_3 - \beta^2 + C_4 \left( \frac{\tau}{\tau + 1} \right)^2 \delta \right\}
\]  

where

\[
C_2 = \log(2I^2),
\]

\[
C_3 = 1 - \log 2,
\]

\[
C_4 = \frac{1}{8} + \log 2.
\]

and, \(\alpha\), the fine structure constant is given by

\[
\alpha = \frac{2\pi e^2}{\hbar c}
\]

where \(\hbar\) is Planck’s constant, \(e\) is the electron charge, \(c\) is the speed of light, \(\nu\) is the velocity of the electron, \(I\) is the mean ionization potential, \(\beta\) is \(\nu/c\), \(\tau\) is the electron kinetic energy in units of the electron rest mass, \(\delta\) is the density effect correction based on polarization effects, and \(Z\) is the average atomic number of the medium. The total energy loss includes radiative losses in addition
to the collisional energy losses.

3.4 Bremsstrahlung

An electron, because it has relatively little mass, can be accelerated by the electric field of a nucleus. Any charge, when accelerated, must radiate energy. This energy is given off in the form of bremsstrahlung photons. Bremsstrahlung radiation is mostly emitted in the forward direction for the electron energy range considered in this thesis. The bremsstrahlung yield varies nearly linearly with energy, and with atomic number as $Z^2$. The ratio of radiative to collisional energy loss is given approximately as

$$\frac{(dE/dx)_{\text{rad}}}{(dE/dx)_{\text{col}}} = \frac{ZE}{800}$$

Radiative energy losses therefore only become significant for higher energy electrons. For example, in lead, Equation 3.8 predicts that the radiative energy loss is approximately equal to the collisional energy loss when the kinetic energy of the electron is about 9.3 MeV. The ratio of radiative to collisional energy loss is also given in Table 85 of the MCNP output.

MCNP samples the probability distributions for the generation of bremsstrahlung photons based on a modified version of the Bethe-Heitler\textsuperscript{21} Born approximation results as described in Koch and Motz\textsuperscript{22}. MCNP samples from tabular data describing bremsstrahlung production probabilities, and photon energy and angular distributions. MCNP samples the bremsstrahlung probabilities at each electron substep. The energy of the bremsstrahlung photon is subtracted from the electron energy at the end of the substep, although bremsstrahlung generation does not explicitly affect the direction of the electron.

The angular distribution for bremsstrahlung photons can also be sampled using a very simple model rather than the detailed probability tables previously described. This simple distribution is given by

$$f(\mu)d\mu = \frac{1 - \beta^2}{2(1 - \beta \mu)^2}d\mu$$

where $\mu = \cos \theta$, the angle between the electron and photon trajectory, $v$ is the velocity of the electron, and $\beta = v/c$. This method of sampling can be invoked by setting the fourth entry on the PHYS:E card to be 1. Note that this method is independent of the material in the transport problem. This method of sampling is explored further in Section 6.1.

3.5 Energy Straggling

An electron energy step is a statistical process, since it includes the overall effect of many random collisions. Probabilistic fluctuations in the electron (or any other charged particle) energy loss rate will therefore occur. That is, a number of electrons under an identical set of material conditions and the same electron energy, will show a distribution of energies as they pass a given depth. As charged particles slow down, it is important to note that the most probable energy loss
will differ from the mean energy loss. The collisional stopping power is based on the mean energy loss. When traveling short distances in matter, the total number of collisions will be small, and the distribution of energies will be quite skewed from the mean energy loss predicted by the stopping power. As the number of collisions increases, the distribution of energy losses assumes a more Gaussian shape.

These straggling effects mandate enhancements to the continuous slowing down approximation (CSDA). As described in Ref. 1, Landau\textsuperscript{16} describes the energy loss distribution under the a set of assumptions, the most important of which is that there be small mean energy loss compared to the electron’s energy. The additions of Blunck and Leisegang\textsuperscript{17} are also included in MCNP. This gives a Landau distribution convoluted with a Gaussian distribution, which is essentially a broadening of the energy loss distribution.

The impact of straggling on electron transport simulations is explored further in this thesis. A series of electron depth dose curves in water are presented in Section 6.6 that include a comparison of straggling and CSDA results.

### 3.6 Knock-On Electrons

Knock-on electrons are electrons scattered by other electrons in impact ionization. These electrons have enough energy to form particle tracks of their own. The differential cross section is given by Møller\textsuperscript{28}. Secondary particles are not tracked in MCNP for energy transfers greater than $\varepsilon_c$, which represents a low energy cutoff. The primary electron is not affected by the generation of a knock-on electron in that its energy and direction are not updated. The multiple scattering theories should adequately account for these effects. The secondary electron is banked with angle and energy as sampled from the Møller cross section. The effect of knock-on electrons is also explored in Section 6.6, as part of an extensive study of the effect of various physics parameters on electron dose in water.
4. Bremsstrahlung Verification Calculations

This portion of the thesis describes a set of thick-target bremsstrahlung calculations. The targets are "thick" in that their thickness is greater than an electron range; the targets are thin to photons. Previous studies on these data have been performed using EGS\textsuperscript{29}, ITS\textsuperscript{20}, and MCNP4A\textsuperscript{30}. MCNP4B simulations of three sets of experiments are described. They are the absolute thick-target bremsstrahlung measurements of Faddegon \textit{et al.}\textsuperscript{2-4} and O'Dell \textit{et al.}\textsuperscript{5}, as well as the relative bremsstrahlung measurements of Starfelt and Koch\textsuperscript{6}.

4.1 Faddegon \textit{et al.} Experiment

4.1.1 Experimental Methods

The most detailed set of the three bremsstrahlung calculations described in this report were the MCNP simulations of the experiments of Faddegon \textit{et al.}\textsuperscript{2-4}. These experiments provided bremsstrahlung spectra and integrated yields from thick targets of Be, Al, and Pb at angles of 0°, 1°, 2°, 4°, 10°, 30°, 60°, and 90° relative to the beam axis for electrons of 15 MeV incident energy. The spectra are absolute in the sense that they are in units of photons per incident electron.

The bremsstrahlung yield, as defined by Faddegon, is the number of photons of energy \( E \) per unit energy from the target which reach a given point \( P \) in a vacuum per unit solid angle per electron incident on the target. The solid angle is defined from the point of intersection of the electron beam axis with the upstream surface of the target. The differential bremsstrahlung yield can be written

\[
\frac{dS}{dE} = \frac{1}{N_e} \frac{d^2N_\gamma(E)}{dEd\Omega},
\]

where the derivative term on the right hand side of Eq. 4.1 is the number of photons with energy between \( E \) and \( E+dE \) which exit the target and reach point \( P \) per unit solid angle, and \( N_e \) is the number of incident electrons. The integrated bremsstrahlung yield can be written

\[
S_{E_0} = \int_{E_0}^{E_{\text{max}}} \frac{dS}{dE} dE,
\]

where \( E_0 \) is the low energy cutoff and \( E_{\text{max}} \) is the maximum photon energy in the spectrum, which is equal to the incident electron energy. Both the experiment and simulations used a low energy cutoff of 145 keV.

The electron beam passed through a thin Ti exit window and a Si beam monitoring detector prior to impinging on the target chamber. The targets were Pb (9.13 g/cm\(^2\) thick, 17.95 g/cm\(^2\) radius), Al (9.74 g/cm\(^2\) thick, 9.81 g/cm\(^2\) radius), and Be (11.67 g/cm\(^2\) thick, 6.72 g/cm\(^2\) radius) cylinders. The targets are thick for electrons, but not for photons. The targets were surrounded by a stainless steel target chamber, except for the 30°, 60°, and 90° measurements. There was an additional Al exit window downstream of the target. The photons then passed through a Pb collimator prior to being collected in a NaI detector.
4.1.2 Monte Carlo Simulation Description

The Monte Carlo simulation was designed to match the experiment as faithfully as possible. See Appendix A.1 and A.2 for sample MCNP input templates. The work of DeMarco\textsuperscript{30}, who performed a similar study using MCNP4A, was used extensively as a reference. The Al target exit window, side walls of the stainless steel target chamber, and Pb collimator were not included in the simulation since the published experimental results are corrected for these factors. The simulations were done in a vacuum, since the experimental data is also corrected for attenuation in air. The target dimensions corresponded exactly to the published values. The thicknesses for the Ti exit window and Si beam monitory system were taken from the published values, although the radial dimensions were estimated. Further uncertainty is introduced in modeling the stainless steel entrance window. In the MCNP model, the stainless steel was defined as 18\% (weight fraction) chromium, 8\% nickel, and 76\% iron. This model was based on typical 304 stainless steel, neglecting the trace impurities.

The bremsstrahlung yields were tallied using cell flux and detector flux tallies. The spectral data over individual energy bins were tallied, although the primary item of interest was the bremsstrahlung yield integrated over all energies. The tallies were multiplied by the square of the source to detector distance (SDD) to convert the tally units from photons per cm\(^2\) to photons per steradian. The SDD of 300 cm is defined from the upstream surface of the target. The cell tallies were based on the union of two cones and two spheres, which forms an annular spherical region. An angular range of 0.5\(^\circ\) and a radial thickness of 1 mm were used. Ring detectors were defined according to the SDD and a ring radius which reproduces the desired angle. Since the geometry is cylindrically symmetric, ring detectors were used rather than point detectors for maximum efficiency. The simulation geometry is shown below in Figure 4.1 for some arbitrary angle \(\theta\).

![Figure 4.2: MCNP Simulation Geometry.](image-url)
Detector and cell flux tallies are calculated in fundamentally different ways. The cell tally for flux is a track length estimate, in which the time integrated flux is estimated by summing $\frac{WT}{V}$, where $W$ is the particle weight, $T$ is the track length of the particle in the cell, and $V$ is the cell volume. Conversely, a detector tally is a deterministic estimate of the flux at a point in space, or in the case of a ring detector tally, at a point sampled from some location on a ring. The detector flux is calculated

$$\Phi(r, E, \mu) = \frac{Wp(\mu)e^{-\lambda}}{2\pi R^2},$$  \hspace{1cm} (4.3)$$

where $2p(\mu)$ is the probability density function at $\mu$, the cosine of the angle between the particle trajectory and the direction to the detector; $R$ is the distance from the source or collision event to the detector; and

$$\lambda = \int_0^R \Sigma t(s)ds,$$  \hspace{1cm} (4.4)$$

which is the total number of mean free paths integrated over the trajectory from the source or collision event to the detector; $\Sigma_t$ is the total macroscopic cross section.

The exponential term of Eq. 4.3 accounts for the attenuation between the present event and the detector point, and a $1/4\pi R^2$ term accounts for the solid angle effect. The $p(\mu)$ term accounts for the probability of scattering toward the detector instead of the direction selected in the random walk. Each contribution to the detector can be thought of as transporting a "pseudoparticle" to the detector.

In addition to the integrated bremsstrahlung yield, the mean energy of the spectra for several angles was calculated. This was done either by taking a flux weighted average over individual energy bins or by dividing a $*F4$ (energy times flux) tally by the $F4$ tally (flux) over the total energy bin.

4.1.3 Results

The integrated bremsstrahlung yields for Pb, Al, and Be are presented Figures 4.2-4.4. These results were obtained using the default electron and photon settings in MCNP4B. Simulations for angles between $0^\circ$ and $10^\circ$ include the stainless steel entrance window, while angles greater than $10^\circ$ had no stainless steel window. This is consistent with the experiment.
Figure 4.3: Integrated Bremsstrahlung Yield vs Angle for Pb.

Figure 4.2 shows that the discrepancies between experiment and simulation are greatest for the forward directed angles and for 90°. It is interesting to note that the detector tally seems to track the experiment better than the cell tally, even though more detailed physics is used for the cell tally for electron photon problems (see Sec. 6.1). The largest difference between experiment and simulation is 16% at 90° for cell tallies, and 13% at 90° for detector tallies. The error bars for the 0° and 90° simulations were generally the largest, because of the low intensity at 90° and small the solid angle at 0°. Table 4.1 gives the tabular data for Al. The numbers in parentheses are the percent errors.
Table 4.1: Integrated Bremsstrahlung Yield vs Angle for Pb

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.640E+00(2.0)*</td>
<td>2.797E+00(0.3)</td>
<td>2.92E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.463E+00(0.8)</td>
<td>2.667E+00(0.3)</td>
<td>2.80E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.255E+00(0.6)</td>
<td>2.380E+00(0.3)</td>
<td>2.48E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.835E+00(0.4)</td>
<td>1.833E+00(0.3)</td>
<td>1.99E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.122E+00(0.4)</td>
<td>1.125E+00(0.3)</td>
<td>1.20E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>4.338E-01(0.4)</td>
<td>4.310E-01(0.5)</td>
<td>4.47E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>1.444E-01(0.5)</td>
<td>1.334E-01(0.5)</td>
<td>1.29E-01(5.0)</td>
</tr>
<tr>
<td>90</td>
<td>6.029E-02(0.7)</td>
<td>5.860E-02(0.7)</td>
<td>5.19E-02(7.0)</td>
</tr>
</tbody>
</table>

*read as 2.640x10^0 with 2.0% error

Figure 4.4: Integrated Bremsstrahlung Yield vs Angle for Al.
Table 4.2: Integrated Bremsstrahlung Yield vs Angle for Al

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.991E+00(1.5)*</td>
<td>3.224E+00(0.2)</td>
<td>3.42E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.802E+00(0.6)</td>
<td>3.045E+00(0.2)</td>
<td>3.21E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.494E+00(0.4)</td>
<td>2.670E+00(0.2)</td>
<td>2.78E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.931E+00(0.3)</td>
<td>2.009E+00(0.2)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.033E+00(0.3)</td>
<td>1.043E+00(0.2)</td>
<td>1.06E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>2.664E-01(0.3)</td>
<td>2.673E-01(0.3)</td>
<td>2.65E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>7.284E-02(0.5)</td>
<td>7.278E-02(0.3)</td>
<td>6.66E-02(6.0)</td>
</tr>
<tr>
<td>90</td>
<td>3.294E-02(0.7)</td>
<td>3.280E-02(0.3)</td>
<td>2.87E-02(6.0)</td>
</tr>
</tbody>
</table>

*read as 2.991x10^0 with 1.5% error

Figure 4.3 shows the integrated bremsstrahlung yields as a function of angle for Al. The tabular data are given in Table 4.2. The largest deviation for the MCNP simulation and experiment is 14% at 90°, for both cell and detector tallies. Figure 4.4 shows the integrated bremsstrahlung yields for Be. The tabular data are given in Table 4.3. In this case, the 90° data agree within statistical error for both cell and detector tallies, but the 0° cell tally differs from experiment by about 15%. For detector tallies for the materials studied, the calculated bremsstrahlung yields agree with experiment within statistics for a 68% confidence interval. For cell tallies for the materials studied, MCNP is usually able to predict the experimental integrated bremsstrahlung yields to within two standard deviations of the experimental and calculational uncertainties.
Figure 4.5: Integrated Bremsstrahlung Yield vs Angle for Be.

Table 4.3: Integrated Bremsstrahlung Yield vs Angle for Be

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.33E+00(1.8)*</td>
<td>2.58E+00(0.2)</td>
<td>2.73E+00(5.1)</td>
</tr>
<tr>
<td>1</td>
<td>2.17E+00(0.7)</td>
<td>2.41E+00(0.2)</td>
<td>2.57E+00(5.1)</td>
</tr>
<tr>
<td>2</td>
<td>1.91E+00(0.5)</td>
<td>2.05E+00(0.2)</td>
<td>2.14E+00(5.1)</td>
</tr>
<tr>
<td>4</td>
<td>1.39E+00(0.4)</td>
<td>1.44E+00(0.2)</td>
<td>1.54E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>5.97E-01(0.4)</td>
<td>6.03E-01(0.3)</td>
<td>6.30E-01(5.1)</td>
</tr>
<tr>
<td>30</td>
<td>9.36E-02(0.6)</td>
<td>9.19E-02(0.3)</td>
<td>9.49E-02(5.1)</td>
</tr>
<tr>
<td>60</td>
<td>2.29E-02(0.9)</td>
<td>2.26E-02(0.3)</td>
<td>2.38E-02(5.9)</td>
</tr>
<tr>
<td>90</td>
<td>1.07E-02(1.2)</td>
<td>1.05E-02(0.3)</td>
<td>1.06E-02(7.0)</td>
</tr>
</tbody>
</table>

*read as 2.332x10^0 with 1.8% error

Figures 4.5 through 4.7 compare experimental and simulation results for the bremsstrahlung energy spectra for lead, aluminum, and beryllium. These plots compare the default MCNP cell tally with experimental data for 10°. The simulations show excellent agreement for each material. These results show that MCNP can accurately calculate both the integrated bremsstrahlung yields as well as the detailed photon energy spectra.
Figure 4.6: Comparison of experimental and MCNP cell tally bremsstrahlung spectra for aluminum at 10°.

Figure 4.7: Comparison of experimental and MCNP cell tally bremsstrahlung spectra for beryllium at 10°.
The mean energy of the bremsstrahlung spectrum for each target was also calculated and compared with the experimental data for a few emission angles. Table 4.4 summarizes the results of these simulations. The numbers in parentheses are the percent errors. The Al and Pb results agreed quite well with experiment, with only the $0^\circ$ data having statistically significant deviations. The Be simulation results did not track the experiment as well as the other materials did; the $0^\circ$, $60^\circ$, $90^\circ$ tallies differed by a few percent outside the $1\sigma$ error bars. This level of agreement is sufficient to form a $68\%$ confidence interval and shows that the calculated mean energies agree with the experiment within statistical uncertainty.
<table>
<thead>
<tr>
<th>Target</th>
<th>Angle</th>
<th>4B cell</th>
<th>4B detector</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>0</td>
<td>2.62 (3.2)</td>
<td>2.68 (0.5)</td>
<td>2.86 (4.1)</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.08 (0.7)</td>
<td>2.04 (0.6)</td>
<td>2.09 (3.4)</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1.14 (1.1)</td>
<td>1.14 (0.9)</td>
<td>1.15 (2.4)</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>0.55 (1.7)</td>
<td>0.55 (0.9)</td>
<td>0.596 (3.0)</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>0.36 (2.3)</td>
<td>0.348 (0.9)</td>
<td>0.379 (2.5)</td>
</tr>
<tr>
<td>Al</td>
<td>0</td>
<td>2.61 (10.5)</td>
<td>2.59 (1.5)</td>
<td>2.74 (3.7)</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.11 (1.9)</td>
<td>2.09 (1.6)</td>
<td>2.17 (3.1)</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1.39 (2.0)</td>
<td>1.38 (1.8)</td>
<td>1.42 (2.9)</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>0.84 (2.7)</td>
<td>0.83 (1.7)</td>
<td>0.83 (3.0)</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>0.55 (3.2)</td>
<td>0.56 (1.6)</td>
<td>0.57 (2.5)</td>
</tr>
<tr>
<td>Pb</td>
<td>0</td>
<td>3.01 (2.8)</td>
<td>3.08 (0.5)</td>
<td>3.22 (3.5)</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.72 (0.7)</td>
<td>2.73 (0.6)</td>
<td>2.77 (3.0)</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>2.216 (0.5)</td>
<td>2.21 (1.0)</td>
<td>2.25 (3.0)</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>1.827 (0.6)</td>
<td>1.84 (1.1)</td>
<td>1.81 (2.8)</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>1.800 (0.8)</td>
<td>1.84 (1.4)</td>
<td>1.84 (2.6)</td>
</tr>
</tbody>
</table>

### 4.2 O’Dell et al. Experiment

#### 4.2.1 Experimental Methods

O’Dell et al.\(^5\) measured the thick-target bremsstrahlung spectra for 5.3 to 20.9 MeV electrons incident on a gold-tungsten target. The bremsstrahlung target was 0.49 g/cm\(^2\) of tungsten followed by 0.245 g/cm\(^2\) of gold. The spectra were measured using a technique based on deuteron photodisintegration. This method is limited to measuring photon energies above 3 MeV\(^6\). The electrons were incident on the bremsstrahlung target, and the resulting photons interact with a secondary D\(_2\)O target, which provides a source of photoneutrons. The neutrons produced above the D(γ,n)p reaction threshold of 2.23 MeV were analyzed using time-of-flight techniques. This gives absolute bremsstrahlung spectra in units of photons per MeV per steradian per incident electron. Figure 4.8, shown below, illustrates the experimental setup.

#### 4.2.2 Monte Carlo Simulation Description

The bremsstrahlung target was modeled as a thin cylinder of tungsten followed by a thin cylinder of gold. Simulations using 10.0 and 20.9 MeV incident electrons were done. The secondary target was modeled with dimensions of 1.25 x 0.25" and 0.5 x 0.25" for the 10.0 and 20.9 measurements, respectively. The photon spectrum was tallied over the entire face of the cell. This is important since the bremsstrahlung yield is fairly sensitive to angle, especially near 0°. Electron and photon low energy cutoffs were set to 4.0 MeV, which mirror the published experimental result. As shown in Figure 4.8, only the electron beam and bremsstrahlung target were

---

29
modeled, with the photons being tallied over the face of the D$_2$O target. See Appendix A.3 for the input template.

Figure 4.9: Experimental setup for O'Dell et al.

4.2.3 Results

Calculated and experimental bremsstrahlung spectra are shown in Figures 4.9 and 4.10 for incident electron energies of 10.0 and 20.9 MeV, respectively. Error bars for the experimental data are based on O’Dell’s estimate that the errors range from 5 to 10%, except at higher photon energies where poor counting statistics further increase the experimental error. There is good overall agreement between calculation and experiment at both energies. All of the points agree within experimental error, with the exception of the very first data point for the incident energy of 10.0 MeV. There also appear to be some minor discontinuities in the MCNP simulations. These are most likely statistical in nature, and are not a reflection of the cross section data. This can be verified by running the simulation for more histories.

Table 4.5 gives the integrated bremsstrahlung yields for the Au/W target at 10.0 and 20.9 MeV. The results for O’Dell were obtained by integrating the published spectra, while the MCNP result was automatically obtained from the cell tally. The results show that MCNP agrees with experiment to within 5%.
Figure 4.10: Bremsstrahlung Energy Spectrum, 10.0 MeV electrons incident on Au/W.

Table 4.5: Integrated Yields for Au/W for O’Dell

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>O’Dell</th>
<th>MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.1826 (23.6,7.5)*</td>
<td>0.1949 (0.93)</td>
</tr>
<tr>
<td>20.9</td>
<td>2.0929 (29.0,7.5)</td>
<td>2.1956 (0.48)</td>
</tr>
</tbody>
</table>

*first number is propagated percent error, second is percent error in each experimental data point
4.3 Starfelt and Koch Experiment

4.3.1 Experimental Methods

Starfelt and Koch\(^6\) have also measured thick target bremsstrahlung spectra. They report photon spectra for 9.66 MeV electrons incident on a tungsten target for 0° and 12°. They used an electron beam from a 50 MeV betatron which passed through a system of Lucite collimators in order to minimize the angular spread of the beam. The electron current in the target was not measured so the spectra are not absolute. The beam was focused on the bremsstrahlung target by an iron-core magnetic lens. Targets were mounted on aluminum rings 1 mm thick with 52 mm inside diameters. The tungsten target was 5.8 g/cm\(^2\) thick. The bremsstrahlung photons pass through an aluminum window, cadmium filter, and lead collimator before impinging on a NaI(Tl) spectrometer. Figure 4.11 illustrates the experimental setup.

---

Figure 4.11: Bremsstrahlung Energy Spectrum, 20.9 MeV electrons incident on Au/W.
4.3.2 Monte Carlo Simulation Description

Since the photon spectra were corrected for collimator effects and photon absorption between target and spectrometer, the only material included in the simulation was the target (see Appendix A.4). Electron and photon cutoff energies were set to 0.4 MeV. Cell and detector tallies were positioned at 0° and 12° using the same method as described in Section 2.1.2. The cell tallies had an angular range of 0.7°, which is consistent with the experimental setup. To reconcile the differences between the relative experimental results and the absolute MCNP calculations the experimental data were normalized to the simulation at the first (lowest) energy bin.

4.3.3 Results

Figures 4.12 and 4.13 give the 0° and 12° bremsstrahlung spectra as a function of photon energy, respectively. The MCNP results are cell tallies. The experimental and MCNP spectral shapes show good agreement for both angles, and in fact agree within statistical uncertainty. The spectra agree particularly well for lower photon energies, which correspond to the highest photon yields. Error bars are not shown for the experimental data, but Starfelt and Koch estimate the uncertainties to range from about 3-4% at 1 MeV to 11-17% at 9 MeV. The experimental errors become quite large for photon energies above 95% of the incident electron energy. Table 4.6 shows a cell and detector comparison for integrated yield. These results are not compared to experiment because the experiment was not an absolute measurement. These results are consistent with the Faddegon comparisons in that the cell tallies are slightly lower than the detector tallies for forward angles. The values in parentheses are percent errors.

Table 4.6: Integrated Yields for tungsten for Starfelt and Koch

<table>
<thead>
<tr>
<th>Angle</th>
<th>Cell</th>
<th>Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.189 (0.9)</td>
<td>1.2615 (0.1)</td>
</tr>
<tr>
<td>12</td>
<td>0.538 (0.1)</td>
<td>0.5417 (0.2)</td>
</tr>
</tbody>
</table>
Figure 4.13: Experimental and calculated bremsstrahlung spectrum at 0° for 9.66 MeV electrons incident on tungsten

Figure 4.14: Experimental and calculated bremsstrahlung spectrum at 12° for 9.66 MeV electrons incident on tungsten
5. Electron Transmission and Backscatter

This section of the thesis describes a series of electron transmission and backscatter comparisons. These calculations provide insight into the fundamental properties of Monte Carlo electron transport.

5.1 Ebert et al. Experiment

5.1.1 Experimental Methods

Ebert et al.\textsuperscript{7} give a tremendous amount of data for 4.0 to 12.0 MeV monoenergetic electrons incident on a variety of solid targets. In this study, a few of the experimental transmission and backscatter experiments have been simulated using MCNP4B.

A beam of electrons of current $I_0$ incident on a planar target is backscattered, absorbed, and transmitted. During some time $\tau$, a charge $Q_0 = I_0 \tau$ is incident on the target. The transmission coefficient $T$ is given by

$$T = Q_T/Q_0 = Q_T/(Q_B + Q_A + Q_T), \quad (5.1)$$

where $Q_T$ is the charge transmitted through the target, $Q_A$ is the charge absorbed in the target, and $Q_B$ is the charge backscattered from the target. The backscatter coefficient $B$ is given by

$$B = Q_B/Q_0 = Q_B/(Q_B + Q_A + Q_T). \quad (5.2)$$

Increasing the target thickness will only increase the backscatter coefficient to a certain limiting value. This is the saturation backscatter coefficient.

In this experiment, the electron beam, generated by a linac, had an energy spread of about 1%. The beam passed through two copper collimators, chosen as a compromise between a low-Z, low density material which would produce a large low energy secondary electron background, and a high Z, high density material which would produce a high bremsstrahlung background. The maximum beam diameter allowed by the collimators was 0.6 cm at the target.

The target chamber contained x-ray shielding, an insulated target holder, two large Faraday cups, and a carbon beam stop in addition to the collimator assembly. The Faraday cups were used to collect the transmitted and backscattered electrons. Bias rings, set to -500 V, were mounted in the Faraday cups to minimize the very low energy secondary electron current. The targets ranged in thickness from about 0.03 to 6.0 g/cm\textsuperscript{2}. The targets were either 2.0 or 8.0 cm in diameter. The larger targets ranged in linear thickness from 0.6 to 3.2 cm. The target dimensions were chosen such that the target radius was greater than the sum of the beam radius and the maximum electron range. This configuration will minimize electron escape through the target sides, and approximate a semi-infinite slab geometry. The experimental geometry is described in Figure 5.1.

5.1.2 Monte Carlo Simulation Description

The experimental geometry was greatly simplified for the MCNP simulations (see Appendix A.5). Only the target was explicitly modeled. The transmission and backscatter coefficients were calculated using current tallies at the target faces. This is much simpler than modeling the Faraday cup geometry, and ensures that there are no tally losses from solid angle effects. The current tallies were divided into two cos(\theta) bins, where \theta is defined relative to the positive surface nor-
mal. The transmission coefficient was calculated by using a \( \theta \) range of 0° to 90°, while the backscatter coefficient used a \( \theta \) range of 90° to 180°. The simulations were done in coupled electron/photon mode, and used the default cutoffs of 1 keV.

Figure 5.1: Geometry for Ebert transmission and backscatter experiments.

5.1.3 Results

Transmission coefficients for 10.2 MeV electrons incident on C, Ag, and U foils of varying thicknesses are presented in Figures 5.2 to 5.4. The experimental results and simulation results using MCNP4B default settings are shown. The simulations agree with experiment with varying degrees of success. The experimental uncertainties are estimated at 2%; Ebert et al. only give errors for transmission coefficients between 0.3 and 0.8.

The silver simulations agree with experiment to the greatest degree. The maximum deviation between the default simulation and experiment is 17%, while most of the transmission coefficients agree within 10%. For the range of transmission coefficients that experimental uncertainties are published, the simulation and experiment agree within statistics. For carbon, the default MCNP simulations disagree with experiment by as much as 90% for the last few data points, although the transmission coefficients for thicknesses less than 3.5 g/cm² differ within 10%. The experimental uncertainties in the transmission coefficients for very thick targets may be quite large, which may help account for these discrepancies. For uranium, default MCNP agrees with experiment within 5-15%.

The next three figures are presented in order of increasing Z. For carbon, the experimental data are lower than the simulation results. As Z increases, the magnitude of the experimental data increases relative to the simulation data. This indicates some trend with Z is present in either the experiment or the Monte Carlo simulation, although it is unclear for which case the trend exists.
Figure 5.2: Comparison of transmission coefficients for 10.2 MeV electrons incident on C foils.

Figure 5.3: Comparison of transmission coefficients for 10.2 MeV electrons incident on Ag foils.
Figure 5.4: Comparison of transmission coefficients for 10.2 MeV electrons incident on U foils.

Table 5.1: Electron Saturation Backscatter Comparison

<table>
<thead>
<tr>
<th>Material</th>
<th>Electron Energy (MeV)</th>
<th>Ebert</th>
<th>Dressel</th>
<th>Tabata</th>
<th>MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>4.0E-03</td>
<td>9.0E-03</td>
<td>3.20E-03</td>
<td>5.846E-03(4.0)*</td>
<td></td>
</tr>
<tr>
<td>Ag</td>
<td>7.4E-02</td>
<td>1.8E-01</td>
<td>7.35E-02</td>
<td>8.465E-02(3.0)</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>1.47E-01</td>
<td>3.3E-01</td>
<td>1.36E-01</td>
<td>1.780E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.0E-03</td>
<td>8.6E-03</td>
<td>4.00E-03</td>
<td>6.122E-03(4.0)</td>
<td></td>
</tr>
<tr>
<td>Ag</td>
<td>9.5E-02</td>
<td>2.0E-01</td>
<td>9.70E-02</td>
<td>1.149E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>1.95E-01</td>
<td>3.8E-01</td>
<td>1.72E-01</td>
<td>2.179E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>6.0E-03</td>
<td>1.0E-02</td>
<td>5.00E-03</td>
<td>6.856E-03(3.0)</td>
<td></td>
</tr>
<tr>
<td>Ag</td>
<td>1.39E-01</td>
<td>2.4E-01</td>
<td>1.29E-02</td>
<td>1.504E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>2.45E-01</td>
<td>4.5E-01</td>
<td>2.28E-01</td>
<td>2.780E-01(1.0)</td>
<td></td>
</tr>
</tbody>
</table>

*read as 5.846x10⁻³ with 4.0% error

Table 5.1 shows the results of the backscatter benchmark calculations. The values in parentheses for the Monte Carlo simulations are the percent errors. The calculations were done for carbon, silver, and uranium foils at incident electron energies of 6.0, 8.0, and 10.2 MeV. Data from Dressel\textsuperscript{32} and Tabata\textsuperscript{33} are also included to show the wide range of experimental values that are in the literature. The default MCNP simulations agree with the Ebert experiment to within 8-20%, with the exception of the values for carbon at 10.2 MeV, which disagree by 46%. The agreement of simulation with experiment for carbon at 10.2 MeV was also relatively poor for the transmission results. The errors for the experimental measurements are about 7-10%. Disregarding this outlying value, the overall agreement is fair, and within 2 σ.
6. Physics Parameter Studies

The main purpose of this section is to present a systematic study of the impact of varying physics parameters on the calculational results. The variations show that the results change in the expected way and show where the calculation is sensitive to the choice of model, indicating possibly fruitful areas of further research and code development. This set of simulations explore several physics and variance reduction models for the experiments of Faddegon et al.\textsuperscript{2-4}, described in Section 4.1.1, and Ebert et al.\textsuperscript{7}, described in Section 5.1.1. The effect of varying several of the physics parameters for electron transport is also explored for calculations of depth dose in a water disk.

6.1 Bremsstrahlung Angular Models

In order to study the impact of different physics models for the angular distribution of bremsstrahlung photons, the MCNP electron physics parameter \( \text{IBAD} \) was varied in several simulations of Faddegon's work. Changing \( \text{IBAD} \) from its default of 0 to 1 switches the detailed bremsstrahlung sampling to a simple approximation. For the detailed treatment of bremsstrahlung, MCNP primarily uses the Bethe-Heitler\textsuperscript{21} Born approximation, based on some of the formulas given in Koch and Motz\textsuperscript{22}. The simple probability distribution, invoked when \( \text{IBAD} = 1 \), is given by

\[
p(\mu)\,d\mu = \frac{1-\beta^2}{2(1-\beta\mu)^2}d\mu,
\]

where \( \mu = \cos\theta \) and \( \beta = v/c \). This simple sampling method is always used for detectors, regardless of the value of \( \text{IBAD} \). Specifying the generation of bremsstrahlung photons to be based on Eq. 6.1 forces the actual transport to be consistent with detector contributions.

Figure 6.1 shows the results of the IBAD comparisons for lead. The experimental results are shown with the MCNP4B results for default and IBAD=1 cell tallies, and default detector tallies. These data are also given in Table 6.1. The numbers in parentheses are percent errors. As expected, the IBAD=1 cell tallies track the detector tallies. Changing IBAD produces no statistically significant difference between detector tallies. This is expected because detector tallies always use the simple bremsstrahlung sampling, regardless of the value of IBAD, and for these problems, which are photon thin, the major detector contribution is from first generation bremsstrahlung photons that undergo very little scatter in the problem. The cell tallies for forward angles increase for the case IBAD=1. The detector tallies for these angles are usually greater than default cell tallies as well. The effect of IBAD decreases as the angle increases. Tables 6.2 and 6.3 give results for the analogous simulations for Al and Be. The results are also plotted in Figure 6.2 and 6.3. The same trends that were seen in MCNP4B simulations were seen with MCNP4A IBAD comparisons, which are given for lead and aluminum in Tables 6.4 and 6.5.
Figure 6.1: Integrated bremsstrahlung yield IBAD comparison for lead.

Table 6.1: Pb Integrated Bremsstrahlung Yield, IBAD Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>4B Cell IBAD=1</th>
<th>4B Detector IBAD=1</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.640E+00(2.0)*</td>
<td>2.797E+00(0.3)</td>
<td>2.822E+00(2.0)</td>
<td>2.799E+00(0.3)</td>
<td>2.92E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.463E+00(0.8)</td>
<td>2.667E+00(0.3)</td>
<td>2.641E+00(0.7)</td>
<td>2.669E+00(0.3)</td>
<td>2.80E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.255E+00(0.6)</td>
<td>2.380E+00(0.3)</td>
<td>2.364E+00(0.6)</td>
<td>2.381E+00(0.3)</td>
<td>2.48E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.835E+00(0.4)</td>
<td>1.883E+00(0.3)</td>
<td>1.892E+00(0.4)</td>
<td>1.885E+00(0.3)</td>
<td>1.99E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.122E+00(0.4)</td>
<td>1.125E+00(0.3)</td>
<td>1.136E+00(0.4)</td>
<td>1.127E+00(0.3)</td>
<td>1.2E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>4.338E-01(0.4)</td>
<td>4.310E-01(0.5)</td>
<td>4.337E-01(0.3)</td>
<td>4.316E-01(0.4)</td>
<td>4.47E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>1.444E-01(0.5)</td>
<td>1.434E-01(0.5)</td>
<td>1.433E-01(0.5)</td>
<td>1.436E-01(0.5)</td>
<td>1.29E-01(5.0)</td>
</tr>
<tr>
<td>90</td>
<td>6.029E-02(0.7)</td>
<td>5.860E-02(0.7)</td>
<td>5.999E-02(0.7)</td>
<td>5.852E-02(0.6)</td>
<td>5.19E-02(7.0)</td>
</tr>
</tbody>
</table>

*read as 2.640x10^0 with 2.0% error
Figure 6.2: IBAD comparison for aluminum.

Table 6.2: Al Integrated Bremsstrahlung Yield, IBAD Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Cell</td>
<td>Detector</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>IBAD=1</td>
<td>IBAD=1</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>2.991E+00(1.5)*</td>
<td>3.224E+00(1.5)</td>
<td>3.245E+00(1.5)</td>
<td>3.225E+00(0.2)</td>
<td>3.42E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.802E+00(0.6)</td>
<td>3.045E+00(0.2)</td>
<td>3.013E+00(0.5)</td>
<td>3.044E+00(0.2)</td>
<td>3.21E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.494E+00(0.4)</td>
<td>2.670E+00(0.2)</td>
<td>2.657E+00(0.4)</td>
<td>2.670E+00(0.2)</td>
<td>2.78E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.931E+00(0.3)</td>
<td>2.009E+00(0.2)</td>
<td>2.007E+00(0.3)</td>
<td>2.010E+00(0.2)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.033E+00(0.3)</td>
<td>1.043E+00(0.2)</td>
<td>1.044E+00(0.3)</td>
<td>1.044E+00(0.2)</td>
<td>1.06E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>2.664E-01(0.3)</td>
<td>2.673E-01(0.3)</td>
<td>2.665E-01(0.3)</td>
<td>2.674E-01(0.3)</td>
<td>2.65E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>7.284E-02(0.5)</td>
<td>7.278E-02(0.3)</td>
<td>7.293E-02(0.5)</td>
<td>7.261E-02(0.3)</td>
<td>6.66E-02(6.0)</td>
</tr>
<tr>
<td>90</td>
<td>3.294E-02(0.7)</td>
<td>3.280E-02(0.3)</td>
<td>3.285E-02(0.7)</td>
<td>3.269E-02(0.3)</td>
<td>2.87E-02(6.0)</td>
</tr>
</tbody>
</table>

*read as 2.991x10^0 with 1.5% error
Figure 6.3: IBAD comparison for beryllium.

Table 6.3: Be Integrated Bremsstrahlung Yield, IBAD Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell Faddegon</th>
<th>4B Detector</th>
<th>4B Cell IBAD=1</th>
<th>4B Detector IBAD=1</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.332E+00(1.8)*</td>
<td>2.588E+00(0.2)</td>
<td>2.557E+00(1.8)</td>
<td>2.587E+00(0.3)</td>
<td>2.73E+00(5.1)</td>
</tr>
<tr>
<td>1</td>
<td>2.176E+00(0.7)</td>
<td>2.412E+00(0.2)</td>
<td>2.395E+00(0.7)</td>
<td>2.411E+00(0.3)</td>
<td>2.57E+00(5.1)</td>
</tr>
<tr>
<td>2</td>
<td>1.917E+00(0.5)</td>
<td>2.058E+00(0.2)</td>
<td>2.034E+00(0.5)</td>
<td>2.059E+00(0.2)</td>
<td>2.14E+00(5.1)</td>
</tr>
<tr>
<td>4</td>
<td>1.390E+00(0.4)</td>
<td>1.444E+00(0.2)</td>
<td>1.439E+00(0.4)</td>
<td>1.445E+00(0.2)</td>
<td>1.54E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>5.977E-01(0.4)</td>
<td>6.030E-01(0.3)</td>
<td>6.023E-01(0.4)</td>
<td>6.036E-01(0.3)</td>
<td>6.30E-01(5.1)</td>
</tr>
<tr>
<td>20</td>
<td>8.159E-02(0.6)</td>
<td>8.278E-02(0.3)</td>
<td>8.252E-02(0.6)</td>
<td>8.272E-02(0.3)</td>
<td>8.69E-02(5.1)</td>
</tr>
<tr>
<td>30</td>
<td>9.368E-02(0.6)</td>
<td>9.195E-02(0.3)</td>
<td>9.214E-02(0.6)</td>
<td>9.202E-02(0.4)</td>
<td>9.49E-02(5.1)</td>
</tr>
<tr>
<td>40</td>
<td>2.294E-02(0.9)</td>
<td>2.265E-02(0.3)</td>
<td>2.251E-02(0.9)</td>
<td>2.261E-02(0.3)</td>
<td>2.38E-02(5.9)</td>
</tr>
<tr>
<td>90</td>
<td>1.079E-02(1.2)</td>
<td>1.053E-02(0.3)</td>
<td>1.044E-02(1.3)</td>
<td>1.048E-02(0.3)</td>
<td>1.06E-02(7.0)</td>
</tr>
</tbody>
</table>

*read as 2.332x10^0 with 1.8% error
Table 6.4: Pb Integrated Bremsstrahlung Yield, MCNP4A IBAD Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4A Cell</th>
<th>4A Detector Cell</th>
<th>4A Cell IBAD=1</th>
<th>4A Detector IBAD=1</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.338E+00(2.7)*</td>
<td>3.356E+00(0.5)</td>
<td>3.412E+00(3.1)</td>
<td>3.349E+00(0.5)</td>
<td>2.92E+00(5.0)2</td>
</tr>
<tr>
<td>1</td>
<td>2.650E+00(1.1)</td>
<td>2.914E+00(0.4)</td>
<td>2.933E+00(1.1)</td>
<td>2.916E+00(0.5)</td>
<td>.80E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.297E+00(0.8)</td>
<td>2.413E+00(0.4)</td>
<td>2.411E+00(0.9)</td>
<td>2.414E+00(0.5)</td>
<td>2.48E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.827E+00(0.6)</td>
<td>1.884E+00(0.4)</td>
<td>1.896E+00(0.7)</td>
<td>1.889E+00(0.5)</td>
<td>1.99E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.134E+00(0.5)</td>
<td>1.140E+00(0.5)</td>
<td>1.133E+00(0.6)</td>
<td>1.138E+00(0.6)</td>
<td>1.2E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>4.369E-01(0.5)</td>
<td>4.374E-01(0.3)</td>
<td>4.410E-01(0.6)</td>
<td>4.375E-01(0.7)</td>
<td>4.47E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>1.470E-01(0.6)</td>
<td>1.464E-01(0.7)</td>
<td>1.458E-01(0.8)</td>
<td>1.476E-01(0.8)</td>
<td>1.29E-01(5.0)</td>
</tr>
<tr>
<td>90</td>
<td>6.107E-02(0.9)</td>
<td>6.028E-02(0.9)</td>
<td>6.026E-02(1.0)</td>
<td>6.015E-02(0.9)</td>
<td>5.19E-02(7.0)</td>
</tr>
</tbody>
</table>

*read as 3.338x10^0 with 2.7% error

Table 6.5: Al Integrated Bremsstrahlung Yield, MCNP4A IBAD Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4A Cell</th>
<th>4A Detector</th>
<th>4A Cell IBAD=1</th>
<th>4A Detector IBAD=1</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.744E+00(2.0)*</td>
<td>3.959E+00(0.3)</td>
<td>3.837E+00(1.7)</td>
<td>3.965E+00(0.3)</td>
<td>3.42E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>3.042E+00(0.7)</td>
<td>3.368E+00(0.3)</td>
<td>3.318E+00(0.6)</td>
<td>3.373E+00(0.3)</td>
<td>3.21E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.522E+00(0.6)</td>
<td>2.695E+00(0.3)</td>
<td>2.698E+00(0.5)</td>
<td>2.698E+00(0.2)</td>
<td>2.78E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.942E+00(0.4)</td>
<td>2.009E+00(0.3)</td>
<td>2.015E+00(0.4)</td>
<td>2.009E+00(0.3)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.045E+00(0.4)</td>
<td>1.057E+00(0.3)</td>
<td>1.060E+00(0.4)</td>
<td>1.056E+00(0.3)</td>
<td>1.06E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>2.723E-01(0.4)</td>
<td>2.710E-01(0.3)</td>
<td>2.733E-01(0.4)</td>
<td>2.712E-01(0.3)</td>
<td>2.65E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>7.416E-02(0.6)</td>
<td>7.408E-02(0.3)</td>
<td>7.404E-02(0.6)</td>
<td>7.397E-02(0.3)</td>
<td>6.66E-02(6.0)</td>
</tr>
<tr>
<td>90</td>
<td>3.367E-02(0.8)</td>
<td>3.362E-02(0.4)</td>
<td>3.343E-02(0.8)</td>
<td>3.353E-02(0.4)</td>
<td>2.87E-02(6.0)</td>
</tr>
</tbody>
</table>

*read as 3.744x10^0 with 2.0% error

6.2 Coherent Scatter

The impact of coherent scatter on tally results was also examined. Table 6.6 shows the integrated yields for lead at a few angles. The yields for angles less than 30° can not be compared to experiment because the simulations did not include the stainless steel entrance window (see Section 4.1.1). The geometry for the two simulations were, however, consistent with each other. The number of histories did differ between the two simulations, so the statistical errors cannot be directly compared. Figure 6.4 compares the bremsstrahlung spectra at 10° for detector tallies with and without coherent scatter. Table 6.6 and Figure 6.4 show that coherent scatter does not significantly affect either the bremsstrahlung spectra or the integrated yield. Coherent scatter can, however, affect the statistical convergence of detector tallies. The detector tallies without coherent scatter passed the MCNP statistical checks for tally convergence much sooner than the simula-
tion with coherent scatter. This is because including coherent scatter can lead to very large detector tally scores, and thus a higher variance. These large scores were verified by a separate calculation, so MCNP is behaving as expected.

Table 6.6: Pb Integrated Bremsstrahlung Yield, Coherent Scatter Comparison

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Cell no coherent scatter</th>
<th>4B Detector</th>
<th>4B Detector no coherent scatter</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.717E+00(2.2)</td>
<td>2.853E+00(3.7)</td>
<td>2.811E+00(0.3)</td>
<td>2.802E+00(0.5)</td>
</tr>
<tr>
<td>1</td>
<td>2.509E+00(0.8)</td>
<td>2.464E+00(1.4)</td>
<td>2.681E+00(0.3)</td>
<td>2.669E+00(0.5)</td>
</tr>
<tr>
<td>2</td>
<td>2.280E+00(0.6)</td>
<td>2.278E+00(1.0)</td>
<td>2.401E+00(0.3)</td>
<td>2.385E+00(0.5)</td>
</tr>
<tr>
<td>4</td>
<td>1.836E+00(0.5)</td>
<td>1.846E+00(0.8)</td>
<td>1.901E+00(0.3)</td>
<td>1.926E+00(0.5)</td>
</tr>
<tr>
<td>10</td>
<td>1.133E+00(0.4)</td>
<td>1.131E+00(0.7)</td>
<td>1.137E+00(0.4)</td>
<td>1.146E+00(0.6)</td>
</tr>
<tr>
<td>30</td>
<td>4.338E-01(0.4)</td>
<td>4.341E-01(0.6)</td>
<td>4.310E-01(0.5)</td>
<td>4.315E-01(0.8)</td>
</tr>
<tr>
<td>60</td>
<td>1.444E-01(0.5)</td>
<td>1.438E-01(0.8)</td>
<td>1.434E-01(0.5)</td>
<td>1.450E-01(0.9)</td>
</tr>
<tr>
<td>90</td>
<td>6.029E-02(0.7)</td>
<td>6.106E-02(1.2)</td>
<td>5.860E-02(0.7)</td>
<td>5.959E-02(1.0)</td>
</tr>
</tbody>
</table>

*read as 2.717x10^0 with 2.2% error

Figure 6.4: Coherent scatter comparison for lead, detector tally.

6.3 Electron sub-step size

The ESTEP parameter, which sets the number of electron substeps per energy step, was also varied for the pre-target material in order to test the existence of bremsstrahlung step size sam-
pling artifacts\textsuperscript{2}. Very thin material regions such as the pre-target Ti exit window, Si detector, and stainless steel target chamber present in this problem may not allow enough electron substeps for an accurate simulation of the electron's trajectory. One of the improvements in MCNP4B over MCNP4A was the mitigation of an electron sub-step artifact for bremsstrahlung production. Comparisons of versions 4B and 4A are presented next.

For MCNP4A, it has been reported that increasing ESTEP will eliminate artificially high bremsstrahlung yields for forward angles\textsuperscript{30}. Figure 6.5 illustrates the effect of increasing ESTEP for two arbitrary electron tracks. In MCNP4A, using the default sub-step size, a bremsstrahlung photon will be sampled either at position 1 or 2, with direction $\Omega_1$ or $\Omega_2$. This means that the photon angular distribution will be very forward peaked, since 50\% of the photons will be in the forward direction. For the case with the increased ESTEP, the same number of photons would be generated, but only 1/7 would be in the forward direction, since any one of $\Omega_1$ through $\Omega_7$ can be sampled. Increasing ESTEP in MCNP4A, therefore, severely impacted the production of bremsstrahlung photons. In MCNP4B, the bremsstrahlung sampling is different in that the code chooses to generate a photon somewhere along the electron substep, and the photon angle is pro-rated according to how far along the substep the photon has been sampled. This will lead to less of a dependence on sub-step size for bremsstrahlung production.

![Default ESTEP](image)

![6X Default ESTEP](image)

Figure 6.5: Increasing ESTEP

The ESTEP parameter was varied for Al and Pb target geometries. Tables 6.7 and 6.8 illustrate the effect of changing ESTEP with MCNP4A and MCNP4B for Al. Note that in MCNP4A, the results appear to converge to the experimental result for an ESTEP of 6 times the default. Increasing the ESTEP parameter to 60 times the default value, however, continues to lower the yield. Increasing ESTEP for MCNP4A, therefore, does not allow the user to approach the correct answer, unless some value of ESTEP that gives a correct answer is chosen by chance. This effect is not seen to such a great extent in MCNP4B because the bremsstrahlung sampling scheme has been modified as described above. For example, when comparing the default and 60 times default ESTEP values, the 0° tallies differ by about 40\% for MCNP4A, but only by about 7\% for version 4B.
Table 6.7: MCNP4A ESTEP Comparison for Al

<table>
<thead>
<tr>
<th>Angle</th>
<th>4A Cell</th>
<th>4A Detector</th>
<th>4A Cell 6X ESTEP</th>
<th>4A Detector 6X ESTEP</th>
<th>4A Cell 60X ESTEP</th>
<th>4A Detector 60X ESTEP</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.744E+00(2.0)*</td>
<td>3.954E+00(0.3)</td>
<td>3.345E+00(3.0)</td>
<td>3.392E+00(0.5)</td>
<td>2.080E+00(3.2)</td>
<td>2.288E+00(0.4)</td>
<td>3.42E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>3.042E+00(0.7)</td>
<td>3.365E+00(0.3)</td>
<td>2.855E+00(0.2)</td>
<td>2.635E+00(0.4)</td>
<td>2.095E+00(0.4)</td>
<td>2.201E+00(0.4)</td>
<td>2.21E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.522E+00(0.6)</td>
<td>2.695E+00(0.3)</td>
<td>2.513E+00(0.9)</td>
<td>2.681E+00(0.4)</td>
<td>1.946E+00(0.8)</td>
<td>1.731E+00(0.4)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.942E+00(0.4)</td>
<td>2.099E+00(0.3)</td>
<td>2.039E+00(0.7)</td>
<td>1.680E+00(0.6)</td>
<td>1.731E+00(0.4)</td>
<td>1.731E+00(0.4)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.045E+00(0.4)</td>
<td>1.057E+00(0.3)</td>
<td>1.061E+00(0.5)</td>
<td>1.050E+00(0.5)</td>
<td>1.057E+00(0.4)</td>
<td>1.057E+00(0.4)</td>
<td>1.06E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>7.273E-01(0.4)</td>
<td>7.270E+01(0.3)</td>
<td>7.270E-01(0.5)</td>
<td>7.270E-01(0.6)</td>
<td>2.745E-01(0.6)</td>
<td>2.782E-01(0.5)</td>
<td>2.65E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>7.416E-02(0.6)</td>
<td>7.408E-02(0.3)</td>
<td>7.532E-02(0.8)</td>
<td>7.365E-02(0.5)</td>
<td>7.615E-02(0.8)</td>
<td>7.474E-02(0.5)</td>
<td>6.66E-02(6.0)</td>
</tr>
<tr>
<td>90</td>
<td>3.367E-02(0.8)</td>
<td>3.362E-02(0.4)</td>
<td>3.399E-02(1.1)</td>
<td>3.360E-02(0.5)</td>
<td>3.374E-02(1.2)</td>
<td>3.370E-02(0.5)</td>
<td>2.87E-02(6.0)</td>
</tr>
</tbody>
</table>

*read as 3.744x100 with 2.0% error

Table 6.8: MCNP4B ESTEP Comparison for Al

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>4B Cell 6X ESTEP</th>
<th>4B Detector 6X ESTEP</th>
<th>4B Cell 60X ESTEP</th>
<th>4B Detector 60X ESTEP</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.991E+00(1.5)*</td>
<td>3.224E+00(0.2)</td>
<td>3.047E+00(1.5)</td>
<td>3.287E+00(0.2)</td>
<td>2.816E+00(1.6)</td>
<td>2.976E+00(0.2)</td>
<td>3.42E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.802E+00(0.6)</td>
<td>3.045E+00(0.2)</td>
<td>2.837E+00(0.5)</td>
<td>3.066E+00(0.2)</td>
<td>2.617E+00(0.6)</td>
<td>2.818E+00(0.2)</td>
<td>3.21E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.494E+00(0.4)</td>
<td>2.670E+00(0.2)</td>
<td>2.484E+00(0.4)</td>
<td>2.672E+00(0.2)</td>
<td>2.353E+00(0.4)</td>
<td>2.498E+00(0.2)</td>
<td>2.78E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.931E+00(0.3)</td>
<td>2.099E+00(0.2)</td>
<td>1.928E+00(0.3)</td>
<td>2.015E+00(0.2)</td>
<td>1.898E+00(0.3)</td>
<td>1.974E+00(0.2)</td>
<td>2.14E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.033E+00(0.3)</td>
<td>1.043E+00(0.2)</td>
<td>1.030E+00(0.3)</td>
<td>1.040E+00(0.2)</td>
<td>1.049E+00(0.3)</td>
<td>1.059E+00(0.2)</td>
<td>1.06E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>7.274E-02(0.6)</td>
<td>7.278E-02(0.3)</td>
<td>7.259E-02(0.5)</td>
<td>7.269E-02(0.3)</td>
<td>7.267E-02(0.5)</td>
<td>7.252E-02(0.3)</td>
<td>6.66E-02(6.0)</td>
</tr>
<tr>
<td>60</td>
<td>3.294E-02(0.7)</td>
<td>3.280E-02(0.3)</td>
<td>3.301E-02(0.7)</td>
<td>3.287E-02(0.3)</td>
<td>3.330E-02(0.7)</td>
<td>3.291E-02(0.3)</td>
<td>2.87E-02(6.0)</td>
</tr>
</tbody>
</table>

*read as 2.991x100 with 1.5% error

Figure 6.6 shows the ratio of calculation to experiment for the Al 0° cell tally for a few multiples of the default ESTEP value. Note how MCNP4B is much less sensitive to ESTEP than MCNP4A.
6.4 Energy Grid Sampling

The DBCN:18 parameter was varied to examine the differences caused by using either the default “MCNP-style” energy indexing algorithm (bin-centered treatment), or by using the nearest group boundary method used by ITS3.0\textsuperscript{20}. All precalculated and tabulated data for electrons are stored on an energy grid whose consecutive energy values obey the ratio

\[ \frac{E_n}{E_{n-1}} = k \]  \hspace{1cm} (6.2)

where \( k = 2^{-1/8} \), which results in an average energy loss per major electron step of 8.3\%\textsuperscript{1}.

The differences between the bin centered and nearest bin are illustrated in Figure 6.7. For the MCNP style bin centered energy grid treatment, if an electron has an energy between the grid boundaries \( E_n \) and \( E_{n-1} \), the electron uses the data from group \( n-1 \). In the nearest bin treatment, if the energy of the electron is between the average group energies \( \bar{E}_n \) and \( \bar{E}_{n-1} \), the data from group \( n-1 \) are used. This is most likely done to account for the fact that the electron is losing energy as it takes a step.
Several comparison studies were done to quantify the effect of the DBCN:18 entry. Tables 6.9 and 6.10 give the default and DBCN:18=1 results for Al and Pb. These simulations were done using MCNP4B.

Table 6.9: DBCN:18 Comparisons for Pb

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector</th>
<th>4B Cell Emulate ITS</th>
<th>4B Detector Emulate ITS</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.640E+00(2.0) *</td>
<td>2.797E+00(0.3)</td>
<td>2.663E+00(2.2)</td>
<td>2.775E+00(0.3)</td>
<td>2.92E+00(5.0)</td>
</tr>
<tr>
<td>1</td>
<td>2.463E+00(0.8)</td>
<td>2.667E+00(0.3)</td>
<td>2.472E+00(0.8)</td>
<td>2.641E+00(0.3)</td>
<td>2.80E+00(5.0)</td>
</tr>
<tr>
<td>2</td>
<td>2.255E+00(0.6)</td>
<td>2.380E+00(0.3)</td>
<td>2.240E+00(0.6)</td>
<td>2.356E+00(0.3)</td>
<td>2.48E+00(5.0)</td>
</tr>
<tr>
<td>4</td>
<td>1.835E+00(0.4)</td>
<td>1.883E+00(0.3)</td>
<td>1.800E+00(0.5)</td>
<td>1.853E+00(0.3)</td>
<td>1.99E+00(5.0)</td>
</tr>
<tr>
<td>10</td>
<td>1.122E+00(0.4)</td>
<td>1.125E+00(0.3)</td>
<td>1.092E+00(0.4)</td>
<td>1.101E+00(0.4)</td>
<td>1.2E+00(5.0)</td>
</tr>
<tr>
<td>30</td>
<td>4.338E-01(0.4)</td>
<td>4.310E-01(0.5)</td>
<td>4.131E-01(0.4)</td>
<td>4.146E-01(0.5)</td>
<td>4.47E-01(5.0)</td>
</tr>
<tr>
<td>60</td>
<td>1.444E-01(0.5)</td>
<td>1.434E-01(0.5)</td>
<td>1.351E-01(0.5)</td>
<td>1.336E-01(0.6)</td>
<td>1.29E-01(5.0)</td>
</tr>
<tr>
<td>90</td>
<td>6.029E-02(0.7)</td>
<td>5.860E-02(0.7)</td>
<td>5.577E-02(0.7)</td>
<td>5.534E-02(0.7)</td>
<td>5.19E-02(7.0)</td>
</tr>
</tbody>
</table>

\*read as 2.640 \times 10^0 with 2.0% error
Using the nearest group energy treatment has a greater effect for larger angles. For cell tallies, the bremsstrahlung yield drops by only 2.7% at 0°, which is within the combined statistical uncertainties of the two tallies. At 90°, however, the nearest group method leads to a decrease in the yield of 7.4%. This effect may occur because the scatter distributions at higher angles are more sensitive to changes in energy. Figure 6.8 shows that emulating ITS gives consistently lower values throughout the spectrum at 90°. At smaller angles, where the integrated yields do not differ significantly, the spectra also agree quite well, as shown in Figure 6.9. In both Figures 6.8 and 6.9, only a portion of the bremsstrahlung spectra are shown for clarity.

Table 6.10 also includes data from a simulation combining the effect of ESTEP set to 60 times the default and DBCN:18=1. Increasing ESTEP effects the DBCN:18=1 results in the same way that it does the default MCNP simulation, i.e. the two parameters act independently and do not counteract each other. The forward angles exhibit the largest effect, with a 7% decrease in the 0° cell tally, and practically no difference at 90°.

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Detector Emulate ITS</th>
<th>4B Cell Emulate ITS</th>
<th>4B Detector Emulate ITS 60X ESTEP</th>
<th>4B Detector Emulate ITS 60X ESTEP</th>
<th>Faddegon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.991E+00(1.5)*</td>
<td>3.224E+00(0.2)</td>
<td>2.909E+00(1.6)</td>
<td>3.179E+00(0.2)</td>
<td>2.705E+00(1.6)</td>
<td>2.929E+00(0.2)</td>
</tr>
<tr>
<td>1</td>
<td>2.802E+00(0.6)</td>
<td>3.045E+00(0.2)</td>
<td>2.791E+00(0.6)</td>
<td>2.994E+00(0.2)</td>
<td>2.577E+00(0.6)</td>
<td>2.762E+00(0.2)</td>
</tr>
<tr>
<td>2</td>
<td>2.494E+00(0.4)</td>
<td>2.670E+00(0.2)</td>
<td>2.423E+00(0.4)</td>
<td>2.624E+00(0.2)</td>
<td>2.299E+00(0.4)</td>
<td>2.448E+00(0.2)</td>
</tr>
<tr>
<td>4</td>
<td>1.931E+00(0.3)</td>
<td>2.009E+00(0.2)</td>
<td>1.889E+00(0.3)</td>
<td>1.963E+00(0.2)</td>
<td>1.843E+00(0.3)</td>
<td>1.91E+00(0.2)</td>
</tr>
<tr>
<td>10</td>
<td>1.033E+00(0.3)</td>
<td>1.043E+00(0.2)</td>
<td>9.924E-01(0.3)</td>
<td>1.001E+00(0.2)</td>
<td>1.009E+00(0.3)</td>
<td>1.01E+00(0.2)</td>
</tr>
<tr>
<td>30</td>
<td>2.664E-01(0.3)</td>
<td>2.673E-01(0.3)</td>
<td>2.505E-01(0.4)</td>
<td>2.498E-01(0.3)</td>
<td>2.504E-01(0.4)</td>
<td>2.495E-01(0.3)</td>
</tr>
<tr>
<td>60</td>
<td>7.284E-02(0.5)</td>
<td>7.278E-02(0.3)</td>
<td>6.733E-02(0.5)</td>
<td>6.697E-02(0.3)</td>
<td>6.687E-02(0.5)</td>
<td>6.670E-02(0.3)</td>
</tr>
<tr>
<td>90</td>
<td>3.294E-02(0.7)</td>
<td>3.280E-02(0.3)</td>
<td>3.050E-02(0.7)</td>
<td>3.020E-02(0.3)</td>
<td>3.055E-02(0.7)</td>
<td>3.032E-02(0.3)</td>
</tr>
</tbody>
</table>

*read as 2.991x10^0 with 1.5% error
Figure 6.8: Bremsstrahlung spectrum at 90° for default MCNP and DBCN18=1 (nearest bin).

Figure 6.9: Bremsstrahlung spectrum at 1° for default MCNP and DBCN18=1 (nearest bin).
The impact of the energy grid treatment was also studied for the electron transmission and reflection calculations. The comparisons for the default simulations were presented in Section 3.1.3. Transmission coefficients for 10.2 MeV electrons incident on C, Ag, and U foils of varying thicknesses, including the DBCN:18 simulations, are presented in Figures 6.10 to 6.12. The DBCN:18 results are consistently lower than the default results. Using the nearest bin treatment most likely results in more electron scattering and energy loss, and therefore less electrons are able to escape the slab. The differences between the two energy bin treatments for carbon are more pronounced than for either silver or uranium. This is probably the result of carbon having a much lower Z than either silver or uranium.

For silver, the DBCN:18 simulation and experiment generally agree to within 5%. This is about a 5% improvement over default MCNP. For carbon, the agreement with experiment when using the nearest bin treatment is much improved, especially for thicker foils. The nearest bin treatment gives agreement with experiment that is usually within about 8%, with the exception of the last few points. For uranium, default MCNP agrees with experiment a few percent better than when setting DBCN:18=1.

![Figure 6.10: Comparison of transmission coefficients for 10.2 MeV electrons incident on C foils.](image-url)
Figure 6.11: Comparison of transmission coefficients for 10.2 MeV electrons incident on Ag foils.
Table 6.11: Electron Saturation Backscatter Comparison

<table>
<thead>
<tr>
<th>Material</th>
<th>Electron Energy (MeV)</th>
<th>Ebert</th>
<th>Dressel</th>
<th>Tabata</th>
<th>MCNP</th>
<th>MCNP DBCN:18=1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>10.2</td>
<td>4.0E-03</td>
<td>9.0E-03</td>
<td>3.20E-03</td>
<td>5.846E-03(4.0)</td>
<td>5.175E-03(4.0)*</td>
</tr>
<tr>
<td>Ag</td>
<td>7.4E-02</td>
<td>1.8E-01</td>
<td>7.35E-02</td>
<td>1.36E-01</td>
<td>8.465E-02(3.0)</td>
<td>7.675E-02(3.0)</td>
</tr>
<tr>
<td>U</td>
<td>1.47E-01</td>
<td>3.3E-01</td>
<td>1.36E-01</td>
<td>1.780E-01(2.0)</td>
<td>1.569E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>8.0</td>
<td>5.0E-03</td>
<td>8.6E-03</td>
<td>4.00E-03</td>
<td>6.122E-03(4.0)</td>
<td>5.547E-03(4.0)</td>
</tr>
<tr>
<td>Ag</td>
<td>9.5E-02</td>
<td>2.0E-01</td>
<td>9.70E-02</td>
<td>1.149E-01(2.0)</td>
<td>1.034E-01(3.0)</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>1.95E-01</td>
<td>3.8E-01</td>
<td>1.72E-01</td>
<td>2.179E-01(2.0)</td>
<td>1.961E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>6.0</td>
<td>6.0E-03</td>
<td>1.0E-02</td>
<td>5.00E-03</td>
<td>6.856E-03(3.0)</td>
<td>6.542E-03(4.0)</td>
</tr>
<tr>
<td>Ag</td>
<td>1.39E-01</td>
<td>2.4E-01</td>
<td>1.29E-02</td>
<td>1.504E-01(2.0)</td>
<td>1.334E-01(2.0)</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>2.45E-01</td>
<td>4.5E-01</td>
<td>2.28E-01</td>
<td>2.780E-01(1.01)</td>
<td>2.581E-01(1.0)</td>
<td></td>
</tr>
</tbody>
</table>

*read as 5.175x10^−3 with 4.0% error

Table 6.11 shows the results of the backscatter benchmark calculations, including the DBCN:18=1 results. The values in parentheses are the percent errors. The two simulations for each material agreed to within 10% of each other. The DBCN:18=1 simulation results were consistently lower than the default MCNP simulations. This is again due to the difference in energy grid sampling which causes less electrons to be able to escape the slab.
The simulations using the nearest bin method for these backscatter calculations agree with experiment to a greater degree than the transmission measurements. The agreement is 1-10%, which is within the combined statistical uncertainties of simulation and experiment, with the exception of the outlying point for carbon at 10.2 MeV.

### 6.5 Splitting Schemes for Bremsstrahlung Production

The effect of bremsstrahlung sampling using the PHYS: E BNUM biasing parameter was explored in some detail. BNUM is a variance reduction tool that specifies the production of BNUM times the analog number of bremsstrahlung photons, each with weight 1/BNUM. Simulations with and without BNUM were compared to verify the consistency of the results and to quantify improvements in the tally Figure-of-Merit (FOM). The FOM, as calculated by MCNP, is given by

\[ FOM = \frac{1}{R^2T} \]  \hspace{1cm} (6.3)

where \( R \) is the relative error, and \( T \) is the computer time used in the MCNP problem. The FOM can be better understood if it is written in the following manner:

\[ T = \frac{1}{R^2FOM} \]  \hspace{1cm} (6.4)

This relation enables one to find the computer time needed to reach a desired value of \( R \). The higher the FOM, the less computer time will be needed to reach the desired tally error. An alternate version of MCNP4B, using a special BNUM patch developed by Adams\(^3\), was also included in the comparison. This patch (see Appendix B) alters the BNUM biasing from producing BNUM identical bremsstrahlung photons to sampling a different bremsstrahlung photon BNUM times.

First, the behavior of BNUM was verified in that it reduced the tally errors while still giving an answer consistent with an analog calculation (BNUM=1). Table 6.12 shows these results for default MCNP, MCNP with BNUM=20, and MCNP with the modified sampling scheme for BNUM. All of the BNUM runs were done with ENUM set to 1/BNUM. The ENUM parameter controls how many photon-induced secondary electrons are produced. This is done to keep the number of electrons in the problem the same as in an analog calculation, thus avoiding excessive computer times. Also, these simulations were all done for the same number of electron histories.
Table 6.12: BNUM Comparisons for PB

<table>
<thead>
<tr>
<th>Angle</th>
<th>4B Cell</th>
<th>4B Cell BNUM=20</th>
<th>4B Detector BNUM=20</th>
<th>4B patch Cell BNUM=20</th>
<th>4B patch Detector BNUM=20</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.638E+00(2.1)*</td>
<td>2.797E+00(0.3)</td>
<td>2.656E+00(1.6)</td>
<td>2.798E+00(0.3)</td>
<td>2.593E+00(0.5)</td>
</tr>
<tr>
<td>1</td>
<td>2.462E+00(0.8)</td>
<td>2.667E+00(0.3)</td>
<td>2.481E+00(0.6)</td>
<td>2.664E+00(0.3)</td>
<td>2.450E+00(0.2)</td>
</tr>
<tr>
<td>2</td>
<td>2.255E+00(0.6)</td>
<td>2.380E+00(0.3)</td>
<td>2.268E+00(0.4)</td>
<td>2.372E+00(0.3)</td>
<td>2.229E+00(0.2)</td>
</tr>
<tr>
<td>4</td>
<td>1.835E+00(0.4)</td>
<td>1.883E+00(0.3)</td>
<td>1.833E+00(0.3)</td>
<td>1.891E+00(0.3)</td>
<td>1.796E+00(0.1)</td>
</tr>
<tr>
<td>10</td>
<td>1.122E+00(0.4)</td>
<td>1.125E+00(0.3)</td>
<td>1.124E+00(0.3)</td>
<td>1.128E+00(0.3)</td>
<td>1.100E+00(0.1)</td>
</tr>
<tr>
<td>30</td>
<td>4.347E-01(0.3)</td>
<td>4.316E-01(0.4)</td>
<td>4.337E-01(0.3)</td>
<td>4.299E-01(0.4)</td>
<td>4.170E-01(0.1)</td>
</tr>
<tr>
<td>60</td>
<td>1.449E-01(0.4)</td>
<td>1.439E-01(0.5)</td>
<td>1.445E-01(0.3)</td>
<td>1.423E-01(0.5)</td>
<td>1.374E-01(0.2)</td>
</tr>
<tr>
<td>90</td>
<td>6.017E-02(0.6)</td>
<td>5.875E-02(0.6)</td>
<td>5.986E-02(0.4)</td>
<td>5.946E-02(0.6)</td>
<td>5.850E-02(0.2)</td>
</tr>
</tbody>
</table>

*read as 2.638x10^0 with 2.1% error

The standard versions of MCNP gives nearly identical results independent of the value BNUM. The patched version does not track the standard version exactly, but the results are generally within 2-3%. The decrease in error is also evident from these data, most notably for the 0° tally. Standard MCNP BNUM sampling reduces the error by a factor of about 1.3, while the modified BNUM gives an improvement of a factor of 4.2.

Figures 6.13 and 6.14 show the effect on the spectral data when using BNUM variance reduction for the 0° cell tally. From both figures it is evident that using BNUM does not significantly alter the tally data. The spectral statistics are greatly improved using the modified BNUM sampling, as shown in Figure 6.14. The improvement in the spectral statistics is not as great when using the standard BNUM sampling. Figures 6.15 and 6.16 show the spectral data for the 2° cell tally. This tally converges much faster than the 0° cell tally, so the improvement in statistics is not as pronounced.
Figure 6.13: A comparison of the Pb bremsstrahlung spectra for default (BNUM=1) and standard BNUM=20 variance reduction for the 0° cell tally.

Figure 6.14: A comparison of the Pb bremsstrahlung spectra for standard and modified BNUM sampling (BNUM=20) variance reduction for the 0° cell tally.
Figure 6.15: A comparison of the Pb bremsstrahlung spectra for default (BNUM=1) and standard BNUM=20 variance reduction for the 2° cell tally.

Figure 6.16: A comparison of the Pb bremsstrahlung spectra for standard and modified BNUM sampling (BNUM=20) variance reduction for the 2° cell tally.
A detailed study of the tally Figures-of-Merit (FOM) was done for the standard and modified BNUM sampling schemes. Simulations were done for BNUM values of 1, 3, 10, 20, 30, and 100. It is speculated that the following trends would be less clear if a thicker target were used and the photons underwent more interactions in the target. Figure 6.17 shows the ratio of the FOM for the modified BNUM sampling scheme to the FOM for the standard scheme. The trends are similar for each angle, although higher gains in the FOM are possible for smaller angles. The FOM are much greater for the patched version of MCNP than for the standard MCNP. This is because the code is sampling over a wide range of angles, rather than at one particular angle. This increases the tally efficiency for the cell tallies, which cover a very small angular range. The ratio the FOM begin to drop off as BNUM increases. This is essentially the result of the tally having already converged, with the additional photons created for higher values of BNUM resulting only in an increase in computer time. Figure 6.18 shows ratio of FOM for the detector tallies. The ratio of FOM for a particular BNUM is inversely proportional to the magnitude of the tally angle. The FOM for detector tallies (see Figure 6.18) behave similar to the cell tallies. The FOM once again level off for high values of BNUM. Again, this results from the fact that the tally has already converged, and additional photons slow down the calculation. Detector tallies tend to converge faster than cell tallies because they are deterministic estimates of flux, rather than the result of actual particle transport to the detector region. Every particle contributes to a detector tally, regardless of splitting in the default code. This is why the detector response to BNUM is opposite to that of the cell tallies in that the ratio of FOM for a particular BNUM is proportional to the tally angle.

Figures 6.19 through 6.22 give the ratio of the FOM for the particular value of BNUM (FOMi) to the FOM for the analog case (FOM1), for either the standard or modified BNUM sampling scheme. For both cell and detector tallies, the modified BNUM sampling always produces a FOM greater than the analog case. For the standard BNUM sampling and detector tallying, however, increasing BNUM usually results in a degradation in the FOM. For standard BNUM sampling, using BNUM should not lead to gains in the FOM since only one photon contributes to the detector tally, regardless of BNUM. Figure 6.21 reinforces this fact in that the FOM decreases as BNUM is increased, since more computer time is being spent tracking the extra photons. A degradation in performance is also the case for standard sampling and cell tallies for BNUM greater than 20.

Figures 6.23 and 6.24 show the actual FOM values for the photon current and flux for the downstream face of the target. Since these are integrated quantities over a large angular range sampling more photons will not greatly improve the FOM. The FOM do change with BNUM because different numbers of photons are escaping out the sides of the target and/or being absorbed in the target.
Figure 6.17: Ratio of modified FOM to standard FOM vs BNUM for photon flux cell tallies

Figure 6.18: Ratio of modified FOM to standard FOM vs BNUM for photon flux detector tallies
Figure 6.19: Ratio of $FOM_i$ to $FOM_1$ vs $BNUM$ for standard splitting; cell tallies.

Figure 6.20: Ratio of $FOM_i$ to $FOM_1$ vs $BNUM$ for modified splitting; cell tallies.
Figure 6.21: Ratio of $FOM_i$ to $FOM_1$ vs BNUM for standard splitting; detector tallies.

Figure 6.22: Ratio of $FOM_i$ to $FOM_1$ vs BNUM for standard splitting sampling; detector tallies.
Figure 6.23: FOM vs BNUM for photon current exiting the downstream face of the target in the forward direction

Figure 6.24: FOM vs BNUM for photon flux tally of photons crossing the downstream face of the target
6.6 20 MeV Electrons in Water

This section of the thesis describes a suite of electron depth dose calculations done with MCNP4xq, a preliminary version of MCNP4B. These calculations were performed before the formal release of MCNP4B, although the two versions are the same in terms of electron physics. Energy deposition is one of the most widely recognized benchmarks for electron calculations. These calculations augment the growing database of electron/photon benchmark calculations.

6.6.1 Simulation Geometry

The 10 cm thick disk was divided into cells 0.5 cm thick. The geometry is illustrated in the figure below. It should be noted that the disk is large in the y and z directions. The input file template is given in Appendix A.6. This problem is quite similar to the benchmarks described by Rogers and Bielajew.35

![Figure 6.25: Depth Dose Geometry](image)

6.6.2 Variation of Parameters

Several parameters were varied for this problem. These parameters, highlighted in the template input file (see Appendix A.6), were selected because they should impact the physics models. The problem was run in mode e, electrons only, or mode e p, electrons and photons. Also, several electron physics card parameters were varied. The IPHOT, ISTRG, and RNOK entries were either entered as 0 or 1. Recall that for the integer parameters, 0 is the default, but RNOK has a default of 1. A zero entry for IPHOT means that electrons will produce photons, while an entry of one means that electrons will not produce photons. For ISTRG=0, the straggling for electron energy loss is sampled, while for ISTRG=1, there is no straggling, and continuous slowing down energy loss is modeled. Knock-on electrons are produced when RNOK=1, but not produced when RNOK=0. The 18th entry in the DBCN card was also varied. For an entry of one, the ITS3.0 energy grid sampling scheme is used, while for an entry of zero the default MCNP energy grid is used. Finally, the ESTEP parameter, which controls the number of electron substeps per energy step, was varied from the default of 3 to 15.

Table 6.13 serves a summary of the parameters used and the output for each run. For the run designated inpdef, all of the input parameters are default values. This input file was run for MCNP version 4a as well as 4xq. The first run listed mirrors the default run except that ESTEP is
set to 15. All other runs were performed with the default value of ESTEP=3.

Table 6.13: Input Parameters

<table>
<thead>
<tr>
<th>Input File</th>
<th>IPHOT</th>
<th>ISTRG</th>
<th>RNOK</th>
<th>DBCN (18)</th>
<th>MODE</th>
</tr>
</thead>
<tbody>
<tr>
<td>inp15</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inpdef</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp01</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp02</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp03</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inpdef</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp06</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp07</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp08</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp09</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp10</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp11</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp12</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp13</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp14</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp15</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp16</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp17</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp18</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp19</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp20</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp21</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp22</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp23</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp24</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp25</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp26</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp27</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp28</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>e</td>
</tr>
<tr>
<td>inp29</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>pe</td>
</tr>
<tr>
<td>inp30</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>e</td>
</tr>
<tr>
<td>inp31</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>pe</td>
</tr>
<tr>
<td>inp32</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>e</td>
</tr>
</tbody>
</table>
6.6.3 Problem Tallies

The main item of interest in this problem was energy deposition, which was tallied with an *F8 tally. A pulse height tally (F8) was used to record the electron and photon energy deposition spectra in each 0.5 cm water cell. The charge deposition in each cell was tallied as well. The electron and photon currents, in terms of weight and energy, were also tallied for each of the water cell surfaces. The electron and photon fluxes were also tallied for each water cell. For electrons, the flux averaged over each of the cells, in terms of weight and energy, was also tallied.

6.6.4 Convergence of Results

Tally fluctuation bins were used to track the convergence of the tallies. For the energy and charge deposition tallies, the last bin (9.5-10 cm depth) was used to check for convergence. For the current (F1) and flux (F2) tallies, the first cosine bin (-1 to 0) and the first surface (x=0.0) were used as tally checks. For the flux averaged over a cell (F4), the last cell was checked (9.5-10 cm depth). These particular bins were chosen because they were deemed to be the least likely to converge. If they converged, then the other bins should definitely converge. In most cases, the tallies passed all ten of the statistical checks. The most common tallies not to pass all of the checks were the electron flux averaged over the last cell, and the charge deposition in the last cell. Of course, there were relatively fewer tallies in these cells, since most of the electrons failed to penetrate that deep into the water. Furthermore, since the tally fluctuation bins were chosen in such a conservative manner, not passing the checks does not necessarily indicate problems with the overall tally.

6.6.5 Results

The graphs presented next show the energy deposition as a function of distance in the water disk. The default values are: electrons will produce photons, sampled straggling for energy loss, knockon electrons are produced, the MCNP energy grid is used, and both electrons and photons are included. The graphs show two curves: the default run, and a run with some parameter(s) different from the default. The title indicates the parameters that differed from the default, as well as the mode of the non-default run.

6.6.6 Timing Studies

It was interesting to note how the cutoff energy affected the speed of the calculation. All of the problems were run with an electron cutoff energy of 189 keV. For comparison purposes, inp02 was run with two other cutoff values. The results are presented in the following table. It should be noted that the speed of the calculation is not linearly related to the cutoff energy of the problem. The figure of merit for the electron energy deposition tally (*F8:e) behaves in a manner quite similar to the particles run per minute.
6.6.7 Observations

A few conclusions can be drawn from the results. For cases with no straggling, there is a slight dose buildup near the incident surface, and much less energy deposited near the end of the slab. These results agree with the no straggling results of Rogers and Bielajew (cf Figure 6.7, Ref. 35), who used EGS4. When knockon electrons are not included, there is more energy deposited early in the water slab, since more energy can be deposited locally and not be carried away by the knockons. This differs slightly from the results of Rogers and Bielajew (cf Figure 6.7, Ref. 35), but is in agreement with the results of Nahum (cf Figure 1.11, Ref. 36). Changing the mode from electrons and photons to electrons only, for any case, tends to increase the energy deposited near the beginning of the slab, and decrease the energy deposited at the end of the slab. This can be explained because in electron mode only, any bremsstrahlung energy is deposited locally, since no photons are created. When the nearest bin energy sampling (used in ITS) energy grid is used, there is more energy deposited early in the water slab, while less energy later in the slab. This implies that there is more scatter in the ITS methodology. For cases where the electrons don’t produce photons, the electron-only mode and the electron and photon mode agree. The CSDA results show that energy is deposited past the electron range of 9.23 cm calculated with the total stopping power because even though collisional straggling is turned off, there is still radiative straggling which can effectively allow the electron to lose less energy due to radiative processes.

<table>
<thead>
<tr>
<th>Cutoff Energy (keV)</th>
<th>Particles per minute</th>
<th>Figure of Merit, *F8:e</th>
</tr>
</thead>
<tbody>
<tr>
<td>189</td>
<td>5495</td>
<td>588</td>
</tr>
<tr>
<td>10</td>
<td>3684</td>
<td>397</td>
</tr>
<tr>
<td>1</td>
<td>2957</td>
<td>319</td>
</tr>
</tbody>
</table>
Figure 6.26: The solid line indicates default settings. The dashed line indicates the same settings, except that there are no knockon electrons. In both cases, the problem includes photons and electrons.

Figure 6.27: The solid line indicates default settings. The dashed line indicates the same settings, except that there are no knockon electrons. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.28: The solid line indicates default settings. The dashed line indicates the same settings, except that there are no knockon electrons, and the ITS energy grid is used. In both cases, the problem includes photons and electrons.

Figure 6.29: The solid line indicates default settings. The dashed line indicates the same settings, except that there are no knockon electrons, and the ITS energy grid is used. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.30: The solid line indicates all default settings. The dashed line indicates all default settings, except the problem only includes electrons.

Figure 6.31: Both runs have default settings, except for ESTEP. The solid line is estep=3 (default) while the dashed line is ESTEP = 15.
Figure 6.32: The solid line indicates default settings. The dashed line indicates the same settings, except that the ITS energy grid is used. In both cases, the problem includes photons and electrons.

Figure 6.33: The solid line indicates default settings. The dashed line indicates the same settings, except that the ITS energy grid is used. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.34: The solid line indicates default settings. The dashed line indicates the same settings, except that there is no straggling, i.e. CSDA energy loss, and no knockon electrons. In both cases, the problem includes photons and electrons.

Figure 6.35: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss, and no knockon electrons. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.36: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss, the ITS energy grid is used, and there are no knockon electrons. In both cases, the problem includes photons and electrons.

Figure 6.37: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss, the ITS energy grid is used, and no knockon electrons. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.38: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss. In both cases, the problem includes photons and electrons.

Figure 6.39: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.40: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss, and the ITS energy grid is used. In both cases, the problem includes photons and electrons.

Figure 6.41: The solid line indicates default settings. The dashed line indicates the same settings, except that there is CSDA energy loss, and the ITS energy grid is used. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.42: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don’t produce photons, and there are no knockon electrons. In both cases, the problem includes photons and electrons.

Figure 6.43: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don’t produce photons, and there are no knockon electrons. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.44: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don’t produce photons, there are no knockon electrons, and the ITS energy grid is used. In both cases, the problem includes photons and electrons.

Figure 6.45: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don’t produce photons, there are no knockon electrons, and the ITS energy grid is used. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.46: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons. In both cases, the problem includes photons and electrons.

Figure 6.47: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.48: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, and the ITS energy grid is used. In both cases, the problem includes photons and electrons.

Figure 6.49: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, and the ITS energy grid is used. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.50: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, there are no knockon electrons, and CSDA energy loss. In both cases, the problem includes photons and electrons.

Figure 6.51: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, there are no knockon electrons, and CSDA energy loss. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
no photons from e-, emulate ITS mode p e
no straggling, no knockon e-

Figure 6.52: The solid line indicates default settings. The dashed line indicates that electrons don’t produce photons, there are no knockon electrons, the ITS energy grid is used, and CSDA energy loss. In both cases, the problem includes photons and electrons.

Figure 6.53: The solid line indicates default settings. The dashed line indicates that electrons don’t produce photons, there are no knockon electrons, the ITS energy grid is used, and CSDA energy loss. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.54: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, and there is CSDA energy loss. In both cases, the problem includes photons and electrons.

Figure 6.55: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, and there is CSDA energy loss. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
Figure 6.56: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, the ITS energy grid is used, and there is CSDA energy loss. In both cases, the problem includes photons and electrons.

Figure 6.57: The solid line indicates default settings. The dashed line indicates the same settings, except that electrons don't produce photons, the ITS energy grid is used, and there is CSDA energy loss. For the default case, the problem includes photons and electrons, while only electrons are included in the other case.
7. Electron Transport Using Macro Monte Carlo

The essential idea in MMC is to define a volume of physical space, termed a "kugel," transport particles, using either condensed history or single event Monte Carlo, through this volume, and tally the particles exiting the volume\textsuperscript{8-11}. This process, performed over many incident energies, can be viewed as a series of local calculations. These tallies are then post-processed to construct a library; the library provides the global information. This library is then used in a new algorithm to transport the particles in a global sense, where the electrons take large-scale, macroscopic kugel steps through the material. The computational acceleration results from the fact that within the kugel there are many interactions which are essentially averaged to produce a net effect, not unlike the condensed history algorithm. Thus, one macro kugel step is equivalent to many electron steps.

As this portion of the thesis developed, several modifications were made to the electron data library to reduce the level of approximation. The data library and transport algorithm developed in this thesis differ from previous work in this area\textsuperscript{8-11}. The next few sections of this thesis trace the development of the library, and gives results that provide insight into the various approximations that were made. The development of the transport algorithm is also described. As a first step, a separate transport code was written to perform the MMC, or kugel, transport as a proof of principle. Then, the MMC algorithm was implemented into a test version of MCNP4B.

7.1 Electron Data Library Generation

7.1.1 Local Calculation

Water was chosen as the material of interest for its relevance in medical physics applications, and since it has been used in previous work\textsuperscript{8-11}. The local calculations were done using MCNP4xq, a preliminary version of 4B\textsuperscript{1}. Many local calculations must be performed in order to generate the library. The structure of the library was originally based on the energy grid given in Table 85 of MCNP output. There are 115 logarithmically spaced energies which, in addition to the default cutoff energy of 1 keV, form the limits of 115 energy groups. Each energy group has a corresponding \textit{drange} value, which is the size of a major energy step in g/cm\textsuperscript{2}. The diameter of the kugel is chosen as the average value of \textit{drange} over that energy group, which is also the average condensed history major step size. For water, there are 3 substeps per major step, so each macro kugel step is equivalent to 3 condensed history substeps. The incident energy for each local calculation is defined as a uniform distribution between the energy limits of each group. Thus, there are 115 MCNP input files needed to generate the proper output, each having the correct kugel diameter and source energy distribution. A sample MCNP input file is included in Appendix C.

The MCNP surface source is used to tally the electrons as the exit the kugel. The surface source file records the position and direction, and energy of the exiting particle. Figure 7.1 below illustrates the local kugel calculation. The surface source file must be converted into a usable ASCII format if it is to be used by the post-processor code (see Appendices D and E).
Incident electron
\[ e^- \]
Exiting electrons
\[ z \]

Figure 7.1: Local Kugel Calculation. The exiting electrons are tallied with the MCNP surface source file.

7.1.2 Exit Angle Bin Distributions

Once the surface source files are in the correct format, the processing code can manipulate the information. The first step is to generate exit angle bin distributions. The code sorts according to exit angle, in terms of \( \cos(\theta) \), to generate equiprobable angular bins, where

\[
\cos(2\theta) = \left( \frac{z-R}{R} \right)
\]

Here, \( R \) is the radius of the kugel. Figure 7.2 illustrates the kugel geometry and how the angle bins divide the kugel. Neither schematic is to scale. Then, based on the desired number of angular bins, the post-processor code generates a file of bin boundaries.

\[ \theta \text{ bin geometry} \]

kugel divided into angle bins

Figure 7.2: Kugel Geometry
Figure 7.3 illustrates the nature of the angular bin distributions for various physics parameters. These distributions are based on 10 equiprobable angular bins, and 20,000 particles, with incident energies uniformly distributed between 18.34 and 20 MeV. The distributions in all three cases are very forward peaked, with only one bin out of ten corresponding to backscattered electrons. Varying the physics parameters only affected the first angular bin, with the addition of knock-on electrons resulting in the smallest possible cos(θ). It was decided that knock-on electrons would not be included in the library, but would instead be treated within MCNP during the global transport calculation. This reduces the computational burden of the local calculation, since transporting knock-on electrons can be quite time consuming. Furthermore, sampled energy straggling was used in the local calculations, rather than the continuous slowing down approximation for energy loss (CSDA). All other physics parameters were set to their default values.

![Comparison of different physics settings](image)

Figure 7.3: A comparison of angle bin distributions for different physics parameters.

In order to ensure that the distributions that were created were in fact correct, separate MCNP verification calculations were performed over the kugel geometry. The kugel was divided into segments representing the angular bin boundaries, and the electron current was tallied over each segment. When the same number of particles are used in the MCNP verification calculation and actual library generation, the data are in perfect agreement. That is, for 10 equiprobable angle bins, 10% of the electrons exit through each bin, as expected.

While using the libraries in preliminary transport calculations, it became evident that using 10 angular bins did not provide enough resolution. The number of bins was increased, therefore, from 10 to 20, 50, and 100. The resulting angular bin distributions for 20 and 100 angular bins are shown in Figure 7.4 and 7.5 for group 1 (18.34 - 20.0 MeV) incident energies and physics settings of energy loss straggling, and no knock-on electrons. Furthermore, 100,000 particles were used in these calculations. Increasing the number of angular bins increases the fraction of forward scattered electrons, since only the first angular bin corresponds to backscattered electrons.
7.1.3 Scattering Angle Distributions

Early research in this study showed that the exit angle described in the previous section was not sufficient to fully describe the direction of the electron as it exited the kugel. At first, the electron was assumed to travel in the direction $\Omega_2$ (see Figure 7.6). Another angle, $\phi$, which describes $\Omega_3$, was therefore, as part of this work, added to the library. The library stores $\cos(\phi)$ values, where

$$\cos \phi = \Omega_2 \cdot \Omega_3$$  \hspace{1cm} (7.6)
All of the information needed to calculate $\Omega_2$, $\Omega_3$ and $\cos(\phi)$ is contained in the surface source file for each local calculation. Figure 7.6 illustrates the kugel geometry and the different electron directions.

![Kugel geometry](image)

Figure 7.6: Kugel geometry, including the new scattering angle $\phi$.

The $\phi$ distributions, similar to the $\theta$ distributions, are very forward peaked. Figure 7.3 shows the $\phi$ distribution for incident energies uniformly distributed between 19.5 and 20.0 MeV (group one). These distributions have been sorted according to $\theta$ bin, i.e. each $\theta$ bin has a corresponding $\phi$ distribution.

![Cos(\phi) distributions](image)

Figure 7.7: Cos($\phi$) distributions for group one energies, separated by $\theta$ bin.

It became evident that a finer bin structure was necessary to describe the rapid rise at the
beginning of the \( \cos(\phi) \) distribution. Dividing the \( \phi \) distribution into 10 equiprobable bins, for example, would lead to errors when sampling from the first bin, since the distribution is not linear in this region. The final bin structure for the \( \phi \) distribution was 10 equiprobable bins, with the first bin divided into 20 “sub-bins,” to more adequately describe the non-linear behavior in this region. If the first \( \phi \) bin is sampled in the transport algorithm, then another random number is chosen and a sub-bin is sampled from within the first bin. This sub-bin structure is only in place for the first bin, since the distributions are relatively linear in the other bins.

Since the \( \theta \) distributions are very similar in shape to the \( \phi \) distributions, it was decided to use the sub-bin structure for the \( \theta \) bins as well. Previously, 100 bins were used to describe the \( \theta \) distribution. This high number of bins was necessary in order to better describe the beginning of the distribution, which rises rapidly to a cosine of 1 and then levels off. When introducing sub-bins, however, this requirement could be relaxed because the sub-bin structure can better describe the beginning of the distribution, and fewer bins are needed to describe the remainder of the distribution, which was more well-behaved.

### 7.1.4 Energy Distributions

The surface source energy information can be manipulated to construct a cumulative probability distribution (CDF) for energy loss within a kugel. The energy distribution was originally based on the MCNP energy grid given in Table 85 of MCNP output. Initially, there were 10 angular bins, each having its own energy distribution. This requirement was relaxed, however, and presently two distributions are calculated. The first distribution is for the electrons that exit in the first \( \theta \) bin, or the “backscattered electrons.” The second distribution encompasses the rest of the electrons. Previously, an energy distribution had been created for each \( \theta \) bin. This, however, proved to be unnecessary, as the energy distributions were not highly correlated with exit angle. The accuracy of the MMC calculation was not adversely affected by this decoupling of angle and energy.

The effects of straggling and knock-on electrons were also examined for the energy distributions. Figure 7.8 shows that there is no significant variation between the continuous slowing down approximation (CSDA) and energy loss straggling. The introduction of knock-on electrons, however, has a significant impact on the distribution, since more low energy electrons are being created. To reiterate, knock-on electrons were not included in the final library. The calculations shown in Figure 7.8 were done using the first of 10 angle bins.

As with the angle bin distributions, the validity of the energy distributions was also checked with MCNP tallies. The tallies were divided into the bin boundaries specified by the post-processing code. The MCNP checks of the energy distribution functions were in perfect agreement with the predictions of the library post-processing code.
As previously described, the initial calculations with 10 angle bins did not provide enough resolution, and 100 angle bins were then used. At the same time, the number of energy distributions was decreased from 10 to 2, since the energy distributions proved to be relatively insensitive to details of the angular binning. These distributions, for group 1 incident energies, are shown in Figure 7.9.

It also became evident that the MCNP energy grid did not provide enough resolution. The energy group structure, therefore, was modified to incorporate finer energy groups (see Appendix
F). The new energy group structure had energy groups of width 0.5 MeV from 20 MeV to 5 MeV. For energies below 5 MeV, the MCNP energy group size is less than 0.5 MeV, so the grid structure was not modified. Changing the energy grid meant that a new set of MCNP local calculations had to be done, leading to a new library. There are 73 energy groups in the new structure, but the energy distributions include lower energies to ensure a completely normalized CDF. There were not as many local calculations, and hence energy groups, because the library was used with a higher low-energy cutoff.

7.1.5 Absorption Probabilities
Occasionally, an electron will undergo a bremsstrahlung event in which it loses a large amount of energy, and thus does not escape from the kugel. These events are termed absorptions. The absorption probabilities are recorded for each local calculation, and comprise the final part of the electron data library. It should be noted that in the original library based on the MCNP energy grid, for the last energy group (lowest incident energies), none of the particles escaped the kugel, so no energy or angle distributions had to be generated for that group.

7.1.6 Creating the Complete Library
The post-processor code is run for each local calculation. A simple input file is used as a command line argument to specify the energy group, the surface source file to be read, and the angle and the energy files to be written. There are in the original library, therefore, 114 angle bin files and 114 energy distribution files. All of these files are merged with files containing the energy group structure, kugel radii, and absorption probabilities to form the complete data library. As discussed previously, the number of angular bins and energy groups were changed, but the method of creating the library remained the same.

Several libraries have been generated; they are summarized in the table below. The "New" energy grid has 0.5 MeV energy groups above 5 MeV, and follows the MCNP grid structure for lower energies. The libraries libpa and libt are different because in libt, each \( \phi \) distribution is correlated with a \( \theta \) bin. In libpa, however, several \( \theta \) bins are averaged when generating \( \phi \) distributions (see Section 4). The library libt is the most up-to-date, and gives the best results.

<table>
<thead>
<tr>
<th>Name</th>
<th>Number of ( \theta ) bins</th>
<th>Number of ( \phi ) bins</th>
<th>Straggling</th>
<th>Energy Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>lib10nos</td>
<td>10</td>
<td>0</td>
<td>No</td>
<td>MCNP</td>
</tr>
<tr>
<td>lib20nos</td>
<td>20</td>
<td>0</td>
<td>No</td>
<td>MCNP</td>
</tr>
<tr>
<td>lib20</td>
<td>20</td>
<td>0</td>
<td>Yes</td>
<td>MCNP</td>
</tr>
<tr>
<td>lib50</td>
<td>50</td>
<td>0</td>
<td>Yes</td>
<td>MCNP</td>
</tr>
<tr>
<td>lib100</td>
<td>100</td>
<td>0</td>
<td>Yes</td>
<td>MCNP</td>
</tr>
<tr>
<td>libnw100</td>
<td>100</td>
<td>0</td>
<td>Yes</td>
<td>New</td>
</tr>
<tr>
<td>libpa</td>
<td>100 + 20 sub-bins</td>
<td>10 + 20 sub-bins</td>
<td>Yes</td>
<td>New</td>
</tr>
<tr>
<td>libt</td>
<td>100 + 20 sub-bins</td>
<td>10 + 20 sub-bins</td>
<td>Yes</td>
<td>New</td>
</tr>
</tbody>
</table>
7.1.7 Calculation Times

The local kugel calculations represented a computer time investment of 60 minutes. This includes 73 local calculations corresponding to the new energy grid structure. Once the final physics parameters were chosen, these local calculations were reused several times to generate the different libraries. An additional 30 minutes was required to format the surface source files. Finally, 65 minutes was needed to run the post-processor code and generate the libraries. In total, 125 minutes of cpu time was invested to create the final data library (libt). All of these calculations were performed on a IBM RS/6000 model 590 workstation. The library generation process represents a one time only investment of computer time, and the library can be reused in many global calculations.

7.1.8 Summary of Final Library

The structure of the final electron data library for kugel transport is as follows. It is based on 73 local calculations for 73 energy groups from 20.0 MeV to 120 keV. The first part of the library lists the equiprobable θ boundaries. The exit angle bins are divided into 20 θ bins for each energy, with the first θ bin divided into 20 sub-bins. Listed next in the library are the energy distributions. These are stored in the form of a cumulative probability distribution function (CDF). The distribution is based on an energy grid containing 114 groups. This distribution extends beyond the 73 energy groups used in the local calculations to ensure a completely normalized distribution for energy loss, and proper energy sampling in the low energy regime. There are two energy CDFs for each energy group. One CDF describes the energy loss in the first, or backscatter, θ bin, while the other CDF describes the energy loss for all other θ bins. The next portion of the library is a listing of the energy group structure and the corresponding kugel radii. The absorption probabilities are listed next. The final portion of the library is the scattering angles. There are 11 cos(θ) bin boundaries listed, corresponding to 10 equiprobable φ bins. There is one φ distribution per θ bin, so the cos(θ) values are listed in a 11 by 20 array, repeated 73 times for each energy group. The first φ bin has been divided into 20 sub-bins, so there is also a 21 by 20 by 73 array containing the sub-bin boundaries for all energies.

7.2 Description of the Macro Monte Carlo Algorithm

This section of the thesis describes the fundamental aspects of the MMC algorithm as it has been implemented in MCNP. The description will be based on the most up-to-date data library, since this library requires the most detailed library and transport algorithm. The MMC algorithm was first implemented in a separate proof of principle transport code. Once it became clear that the algorithm held promise, it was fully implemented into MCNP itself. This patch is included with additional comments in Appendix G. The new variables and their memory allocation are also described in Appendix G.

The MMC kugel option is invoked in the MCNP input file by setting the first IDUM entry to be a non-zero integer. When this option is invoked, a call is made to a new subroutine, RDLIB, from the existing MCNP subroutine XACT, which handles all of the cross section information. The subroutine RDLIB reads in the electron data library from a text file. A message is written to the output file letting the user know that the kugel library has been read in.
The MCNP electron transport subroutine ELECTR has been modified to perform the actual kugel transport. The MMC algorithm utilizes some of the existing parts of ELECTR in addition to adding new code to the subroutine. A simple flowchart, included in Figure 7.10, illustrates the MMC transport algorithm. The first step in the transport is to find the correct kugel energy group, which sets pointers for sampling the energy and angle distributions. The exit angle, $\Theta$, is then sampled, and the direction of the electron is updated. The radius of the kugel is found based on the electron energy, and the distance traveled in the kugel ($z_l$) is calculated based on the exit angle and kugel radius $R_g$:

$$z_l = 2R_g \cos\Theta$$  (7.1)

The MCNP variable $\text{pmf}$, which corresponds to the distance to next collision, is set to $z_l$. The distance to the next cell boundary, $\text{dl}\text{s}$, is calculated next, and the track length in the cell is tallied. A boundary crossing will occur if $\text{pmf}$ is greater than $\text{dl}\text{s}$. The absorption probabilities are then sampled, with the probabilities being scaled as follows. For boundary crossings,

$$P'_g = \frac{\text{dl}\text{s}}{D_g} P_g$$  (7.2)

where $D_g$ is the kugel diameter, $g$ is the energy group, and $P_g$ and $P'_g$ are the unscaled and scaled absorption probabilities, respectively. If no boundary crossing occurs,

$$P'_g = \frac{z_l}{D_g} P_g.$$  (7.3)

If absorbed, the electron is treated as having its energy falling below the cutoff, and the track is terminated. If the electron is not absorbed, a new energy is sampled, and the energy group is updated. If this energy is less than the cutoff, the track is terminated.

The next step in the transport process is to update the position of the electron to either the surface that it crossed in the case of boundary crossing, or to the end of its macro step. Now, a scattering angle, $\Phi$, is sampled, and the direction of the electron is updated once again. The scattering angle is also scaled for boundary crossings using the following assumption:

$$\frac{\text{dl}\text{s}}{\text{pmf}} (\cos\Phi)' = (\cos\Phi)'_{\text{pmf}} \quad \text{for} \quad \cos\Phi \geq 0$$  (7.4)

$$\frac{\text{dl}\text{s}}{\text{pmf}} (\cos\Phi)' = -\left|\cos\Phi\right|_{\text{dl}\text{s}} \quad \text{for} \quad \cos\Phi < 0.$$  (7.5)

The scaling must be split into two cases to avoid getting imaginary results from scaling negative $\cos(\Phi)$ values. The scaling used in Eq. (7.4) and (7.5) are approximations, and not based on any theory. The $\cos\Phi$ distributions are very forward peaked, and the scaling serves to set $\cos\Phi$ closer to 1.0 if the electron’s path in the kugel is cut short by a boundary crossing. After sampling the scattering angle, the electron track continues and the process is repeated. For boundary crossings, the
electron is placed logically in the next cell before the track can continue.

The existing MCNP tally structure has been used to tally energy deposition. When the electron crosses a surface, the energy times the weight of the particle is subtracted from the account of the cell that it is leaving and is added to the account of the cell that it is entering.
Figure 7.10: Flowchart for MMC algorithm
7.3 MMC Results

Several depth dose curves are presented to illustrate the evolution of the data library and show what the requirements for accurate simulation are in the MMC method. See Appendix H for a sample input file used in these calculations. These are followed by more in-depth comparisons of MCNP and MMC for the final library. It should be noted that these calculations are run in electron mode only, and knock-on electrons are not produced. Figure 7.11 shows a few iterations of library development. The first MMC iteration was for 10 equiprobable $\cos(\theta)$ angular bins, with a coarse energy grid structure. This curve clearly shows the need for more forward scattering, since very few electrons are penetrating to the rear of the slab. The next iteration is for 100 angular bins and the same energy grid. The improvements in the forward scattering are clearly evident. The third MMC iteration used 100 angular bins but modified the energy grid, as described in Section 2.2.3. Again, the results show improvement, but still do not satisfactorily agree with the MCNP results.

![Incident Electron Energies distributed between 19.5 and 20.0 MeV](image)

Figure 7.11: Assorted depth dose curves showing improvements to the electron library.

Some additional modifications were implemented in the library which served to further improve the results. The modified MMC results, MCNP results, and the best MMC results from Figure 7.11 are shown in Figure 7.12. Note that the agreement between MMC and MCNP has improved once again. The $\cos(\theta)$ scattering cosines have been added to the library. The distributions as they were implemented in this iteration were not completely correlated with the exit angle $\theta$. Figure 7.7 shows there is some correlation of $\phi$ with $\theta$. Table 7.2 shows how $\cos(\phi)$ was correlated with $\cos(\theta)$ for this first implementation of $\cos(\phi)$ into the library. Recall that there are 100 $\cos(\theta)$ bins. There is some distribution of $\phi$ values for each $\theta$ bin. For the first iteration, the first $\phi$ distribution was calculated from $\phi$ values from the first $\theta$ bin. The second $\phi$ distribution was calcu-
lated from $\phi$ values from the second through the fifth $\theta$ bin. This averaging over several $\theta$ bins continued according to the values given in Table 7.2. Also, this modification to the data library incorporated the sub-bin structure for $\theta$ and $\phi$ as described in Section 7.1.3.

![Incident Electron Energies distributed between 19.5 and 20.0 MeV](image)

Figure 7.12: Modifying the angular distributions had improved the agreement in depth dose.

<table>
<thead>
<tr>
<th>$\phi$ distribution</th>
<th>Range of $\theta$ bins</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2-5</td>
</tr>
<tr>
<td>3</td>
<td>6-10</td>
</tr>
<tr>
<td>4</td>
<td>11-50</td>
</tr>
<tr>
<td>5</td>
<td>51-100</td>
</tr>
</tbody>
</table>

Table 7.2: Initial correlation of $\phi$ with $\theta$

The final improvement in the electron data library is seen in Figure 7.13. The incident energies are distributed between 19.5 and 20.0 MeV. The major modification for this iteration of the library was exactly correlating $\phi$ with $\theta$. Each $\theta$ bin now has a corresponding set of equiprobable $\phi$ bins. There is no longer any averaging over $\theta$. This update proved to provide the necessary accuracy to produce satisfactory agreement between MMC and MCNP, as shown in Figure 7.13. There is generally excellent agreement between MMC and MCNP for all tallies. The x-axis corresponds to the cell tally bin. Each bin corresponds to a water thickness of 0.5 cm. Table 7.3 gives the numerical results for these calculations. The numbers in parentheses are the percent errors. The maximum percent difference between MMC and MCNP for depths less than 9.5 cm is 4%. There
is an 11\% difference between MCNP and MMC for the last tally bin, corresponding to depths between 9.5 and 10.0 cm. The magnitude of the dose has dropped off severely for this bin, which leads to a larger disagreement between MCNP and MMC.

Figure 7.13: Depth Dose for electrons with energy distributed between 19.5 and 20 MeV incident on water. Each cell is 0.5 cm thick.
Table 7.3: Depth Dose for 19.5 to 20 MeV electrons incident on water.

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>MCNP (MeV/incident electron)</th>
<th>MMC (MeV/incident electron)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>1.18042E+00 (0.33)*</td>
<td>1.16697E+00 (0.29)</td>
<td>1.14</td>
</tr>
<tr>
<td>1.0</td>
<td>1.16669E+00 (0.32)</td>
<td>1.16603E+00 (0.29)</td>
<td>0.06</td>
</tr>
<tr>
<td>1.5</td>
<td>1.16027E+00 (0.30)</td>
<td>1.16939E+00 (0.28)</td>
<td>0.79</td>
</tr>
<tr>
<td>2.0</td>
<td>1.17010E+00 (0.29)</td>
<td>1.17525E+00 (0.28)</td>
<td>0.44</td>
</tr>
<tr>
<td>2.5</td>
<td>1.14722E+00 (0.27)</td>
<td>1.17377E+00 (0.27)</td>
<td>2.31</td>
</tr>
<tr>
<td>3.0</td>
<td>1.15171E+00 (0.26)</td>
<td>1.17447E+00 (0.26)</td>
<td>1.98</td>
</tr>
<tr>
<td>3.5</td>
<td>1.14831E+00 (0.24)</td>
<td>1.16083E+00 (0.26)</td>
<td>1.09</td>
</tr>
<tr>
<td>4.0</td>
<td>1.15022E+00 (0.23)</td>
<td>1.15659E+00 (0.24)</td>
<td>0.55</td>
</tr>
<tr>
<td>4.5</td>
<td>1.14858E+00 (0.21)</td>
<td>1.14895E+00 (0.24)</td>
<td>0.03</td>
</tr>
<tr>
<td>5.0</td>
<td>1.15972E+00 (0.22)</td>
<td>1.14370E+00 (0.23)</td>
<td>1.38</td>
</tr>
<tr>
<td>5.5</td>
<td>1.16882E+00 (0.21)</td>
<td>1.15138E+00 (0.22)</td>
<td>1.49</td>
</tr>
<tr>
<td>6.0</td>
<td>1.17112E+00 (0.22)</td>
<td>1.15527E+00 (0.22)</td>
<td>1.35</td>
</tr>
<tr>
<td>6.5</td>
<td>1.15957E+00 (0.23)</td>
<td>1.14402E+00 (0.23)</td>
<td>1.34</td>
</tr>
<tr>
<td>7.0</td>
<td>1.12126E+00 (0.24)</td>
<td>1.10942E+00 (0.24)</td>
<td>1.06</td>
</tr>
<tr>
<td>7.5</td>
<td>1.04050E+00 (0.27)</td>
<td>1.02381E+00 (0.26)</td>
<td>1.60</td>
</tr>
<tr>
<td>8.0</td>
<td>9.04034E+00 (0.31)</td>
<td>8.85695E+01 (0.30)</td>
<td>2.03</td>
</tr>
<tr>
<td>8.5</td>
<td>7.15802E+00 (0.37)</td>
<td>6.90335E+01 (0.37)</td>
<td>3.56</td>
</tr>
<tr>
<td>9.0</td>
<td>4.90952E+00 (0.48)</td>
<td>4.68934E+01 (0.49)</td>
<td>4.48</td>
</tr>
<tr>
<td>9.5</td>
<td>2.66129E+00 (0.68)</td>
<td>2.60425E+00 (0.69)</td>
<td>2.14</td>
</tr>
<tr>
<td>10.0</td>
<td>1.01815E+00 (1.10)</td>
<td>1.13410E+00 (1.06)</td>
<td>11.39</td>
</tr>
</tbody>
</table>

*read as 1.18042x10^0 with 0.33% error

Table 7.4 gives MMC and MCNP results for the same incident energies but with 1.0 cm thick tally bins. These results show that increasing the bin thickness improves the accuracy of the MMC algorithm. Thicker bins result in less boundary crossings, which lessens the impact of some of the boundary crossing approximations made in the MMC transport.

Table 7.4: Depth Dose for 19.5 to 20 MeV electrons incident on water; coarser bin structure.

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>MCNP (MeV/incident electron)</th>
<th>MMC (MeV/incident electron)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>2.35314E+00 (0.23)*</td>
<td>2.34052E+00 (0.22)</td>
<td>0.54</td>
</tr>
<tr>
<td>2.0</td>
<td>2.32164E+00 (0.21)</td>
<td>2.33230E+00 (0.21)</td>
<td>0.46</td>
</tr>
<tr>
<td>3.0</td>
<td>2.29811E+00 (0.19)</td>
<td>2.30196E+00 (0.20)</td>
<td>0.17</td>
</tr>
<tr>
<td>4.0</td>
<td>2.29925E+00 (0.17)</td>
<td>2.30559E+00 (0.18)</td>
<td>0.28</td>
</tr>
<tr>
<td>5.0</td>
<td>2.30674E+00 (0.16)</td>
<td>2.29041E+00 (0.17)</td>
<td>0.71</td>
</tr>
<tr>
<td>6.0</td>
<td>2.32736E+00 (0.17)</td>
<td>2.29073E+00 (0.17)</td>
<td>1.57</td>
</tr>
<tr>
<td>7.0</td>
<td>2.26714E+00 (0.19)</td>
<td>2.24330E+00 (0.18)</td>
<td>1.05</td>
</tr>
<tr>
<td>8.0</td>
<td>1.94202E+00 (0.23)</td>
<td>1.94022E+00 (0.23)</td>
<td>0.09</td>
</tr>
<tr>
<td>9.0</td>
<td>1.22219E+00 (0.34)</td>
<td>1.21540E+00 (0.34)</td>
<td>0.56</td>
</tr>
<tr>
<td>10.0</td>
<td>3.83116E-01 (0.67)</td>
<td>3.97125E-01 (0.67)</td>
<td>3.66</td>
</tr>
</tbody>
</table>

*read as 2.35314x10^0 with 0.23% error
Table 7.5 gives bulk energy deposition results for electrons of the same incident energies. These problems were defined with one cell forming the entire thickness of water, so no boundary crossings take place except for when electrons escape out the ends of the slab. All of the MMC results agree with MCNP to within 2%.

Table 7.5: Comparison of Bulk Energy Deposition Calculations.

<table>
<thead>
<tr>
<th>Thickness (cm)</th>
<th>MCNP</th>
<th>MMC</th>
<th>Percent Difference</th>
<th>FOM Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>1.1794 (0.33)</td>
<td>1.1583 (0.29)</td>
<td>1.79</td>
<td>1.95</td>
</tr>
<tr>
<td>1.0</td>
<td>2.3508 (0.23)</td>
<td>2.3265 (0.21)</td>
<td>1.04</td>
<td>1.66</td>
</tr>
<tr>
<td>2.0</td>
<td>4.6560 (0.15)</td>
<td>4.6586 (0.16)</td>
<td>0.06</td>
<td>1.45</td>
</tr>
<tr>
<td>4.0</td>
<td>9.2289 (0.10)</td>
<td>9.2458 (0.10)</td>
<td>0.18</td>
<td>1.52</td>
</tr>
<tr>
<td>8.0</td>
<td>18.056 (0.03)</td>
<td>17.958 (0.04)</td>
<td>0.54</td>
<td>1.70</td>
</tr>
</tbody>
</table>

The increased speed in the MMC calculation can be measured by comparing the MMC tally Figure-of-Merit (FOM) with the MCNP FOM. The FOM, as calculated by MCNP, is given by

\[ FOM = \frac{1}{R^2T} \]  \hspace{1cm} (7.6)

where \( R \) is the relative error, and \( T \) is the computer time used in the MCNP problem. The FOM can be better understood if it is written in the following manner:

\[ T = \frac{1}{R^2FOM} \]  \hspace{1cm} (7.7)

This relation enables one to find the computer time needed to reach a desired value of \( R \). The higher the FOM, the less computer time will be needed to reach the desired tally error. Table 7.5 shows that the gain in speed ranges from a factor of 1.45 to 1.95.

Figure 7.14 and Table 7.6 show a comparison of MCNP and MMC results for energies between 14.5 and 15.0 MeV. Each tally bin corresponds to a thickness of 0.4 cm. Again, the MMC algorithm gives good agreement with MCNP, as the tallies agree within 6%, except for the last tally bin where the dose has become small. Figures 7.15 and 7.16 show comparisons of the MMC and MCNP results for electrons of energy 9.5 to 10.0 MeV and 4.5 to 5.0 MeV, respectively. These data are also given in Tables 7.7 and 7.8. The agreement of MMC with MCNP worsens as energy decreases. Most of the tallies agree within 6-10% for these energies, but there also a few tallies that diverge by 20-30% for doses of small magnitude, which correspond to greater depths in the slab. Electrons in these regions will have low energies, which could account for the increased deviation between the MMC and MCNP results.
Figure 7.14: Depth Dose for electrons with energy distributed between 14.5 and 15 MeV incident on water. Each cell is 0.4 cm thick.

Table 7.6: Depth Dose for 14.5 to 15 MeV electrons incident on water.

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>MCNP (MeV/incident electron)</th>
<th>MMC (MeV/incident electron)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>8.86999E-01 (0.29) *</td>
<td>8.77971E-01 (0.27)</td>
<td>1.02</td>
</tr>
<tr>
<td>0.8</td>
<td>8.96879E-01 (0.28)</td>
<td>8.95222E-01 (0.26)</td>
<td>0.18</td>
</tr>
<tr>
<td>1.2</td>
<td>8.84273E-01 (0.26)</td>
<td>9.06295E-01 (0.26)</td>
<td>2.49</td>
</tr>
<tr>
<td>1.6</td>
<td>8.90686E-01 (0.25)</td>
<td>9.09748E-01 (0.26)</td>
<td>2.14</td>
</tr>
<tr>
<td>2.0</td>
<td>8.89649E-01 (0.23)</td>
<td>9.13602E-01 (0.26)</td>
<td>2.69</td>
</tr>
<tr>
<td>2.4</td>
<td>8.97186E-01 (0.23)</td>
<td>9.08534E-01 (0.25)</td>
<td>1.26</td>
</tr>
<tr>
<td>2.8</td>
<td>9.07823E-01 (0.21)</td>
<td>9.01303E-01 (0.24)</td>
<td>0.72</td>
</tr>
<tr>
<td>3.2</td>
<td>9.22503E-01 (0.21)</td>
<td>9.06365E-01 (0.23)</td>
<td>1.75</td>
</tr>
<tr>
<td>3.6</td>
<td>9.37261E-01 (0.21)</td>
<td>9.19077E-01 (0.22)</td>
<td>1.94</td>
</tr>
<tr>
<td>4.0</td>
<td>9.57684E-01 (0.21)</td>
<td>9.42134E-01 (0.22)</td>
<td>1.62</td>
</tr>
<tr>
<td>4.4</td>
<td>9.65952E-01 (0.22)</td>
<td>9.69306E-01 (0.22)</td>
<td>0.35</td>
</tr>
<tr>
<td>4.8</td>
<td>9.67522E-01 (0.23)</td>
<td>9.66219E-01 (0.22)</td>
<td>0.13</td>
</tr>
<tr>
<td>5.2</td>
<td>9.30365E-01 (0.24)</td>
<td>9.33531E-01 (0.24)</td>
<td>0.34</td>
</tr>
<tr>
<td>5.6</td>
<td>8.66531E-01 (0.27)</td>
<td>8.47455E-01 (0.26)</td>
<td>2.20</td>
</tr>
<tr>
<td>6.0</td>
<td>7.41326E-01 (0.31)</td>
<td>7.16468E-01 (0.31)</td>
<td>3.35</td>
</tr>
<tr>
<td>6.4</td>
<td>5.72823E-01 (0.38)</td>
<td>5.38478E-01 (0.39)</td>
<td>6.00</td>
</tr>
<tr>
<td>6.8</td>
<td>3.74396E-01 (0.50)</td>
<td>3.49098E-01 (0.52)</td>
<td>6.76</td>
</tr>
<tr>
<td>7.2</td>
<td>1.87362E-01 (0.74)</td>
<td>1.83003E-01 (0.76)</td>
<td>2.33</td>
</tr>
<tr>
<td>7.6</td>
<td>5.97434E-02 (1.29)</td>
<td>7.53410E-02 (1.19)</td>
<td>26.11</td>
</tr>
</tbody>
</table>

*read as 8.86999x10^-1 with 0.29% error
9.5 to 10 MeV electrons

Figure 7.15: Depth Dose for electrons with energy distributed between 9.5 and 10 MeV incident on water. Each cell is 0.3 cm thick.

Table 7.7: Depth Dose for 9.5 to 10 MeV electrons incident on water.

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>MCNP (MeV/incident electron)</th>
<th>MMC (MeV/incident electron)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>6.19903E-01 (0.23)*</td>
<td>6.20086E-01 (0.25)</td>
<td>0.03</td>
</tr>
<tr>
<td>0.6</td>
<td>6.33841E-01 (0.23)</td>
<td>6.55579E-01 (0.24)</td>
<td>3.43</td>
</tr>
<tr>
<td>0.9</td>
<td>6.36491E-01 (0.22)</td>
<td>6.63956E-01 (0.23)</td>
<td>4.32</td>
</tr>
<tr>
<td>1.2</td>
<td>6.43641E-01 (0.21)</td>
<td>6.69377E-01 (0.23)</td>
<td>4.00</td>
</tr>
<tr>
<td>1.5</td>
<td>6.56539E-01 (0.20)</td>
<td>6.80375E-01 (0.23)</td>
<td>3.63</td>
</tr>
<tr>
<td>1.8</td>
<td>6.81108E-01 (0.20)</td>
<td>6.94717E-01 (0.22)</td>
<td>2.00</td>
</tr>
<tr>
<td>2.1</td>
<td>7.06333E-01 (0.21)</td>
<td>7.13949E-01 (0.21)</td>
<td>1.05</td>
</tr>
<tr>
<td>2.4</td>
<td>7.32582E-01 (0.21)</td>
<td>7.40331E-01 (0.21)</td>
<td>1.06</td>
</tr>
<tr>
<td>2.7</td>
<td>7.59068E-01 (0.22)</td>
<td>7.58889E-01 (0.22)</td>
<td>0.02</td>
</tr>
<tr>
<td>3.0</td>
<td>7.65269E-01 (0.23)</td>
<td>7.62473E-01 (0.22)</td>
<td>0.37</td>
</tr>
<tr>
<td>3.3</td>
<td>7.44053E-01 (0.24)</td>
<td>7.34352E-01 (0.24)</td>
<td>1.30</td>
</tr>
<tr>
<td>3.6</td>
<td>6.87480E-01 (0.27)</td>
<td>6.68897E-01 (0.26)</td>
<td>2.70</td>
</tr>
<tr>
<td>3.9</td>
<td>5.86653E-01 (0.31)</td>
<td>5.51728E-01 (0.31)</td>
<td>5.95</td>
</tr>
<tr>
<td>4.2</td>
<td>4.43631E-01 (0.38)</td>
<td>3.98223E-01 (0.40)</td>
<td>10.24</td>
</tr>
<tr>
<td>4.5</td>
<td>2.79506E-01 (0.51)</td>
<td>2.34142E-01 (0.57)</td>
<td>16.23</td>
</tr>
<tr>
<td>4.8</td>
<td>1.29108E-01 (0.78)</td>
<td>1.07106E-01 (0.88)</td>
<td>17.04</td>
</tr>
<tr>
<td>5.1</td>
<td>3.65983E-02 (1.45)</td>
<td>3.50225E-02 (1.53)</td>
<td>4.31</td>
</tr>
<tr>
<td>5.4</td>
<td>4.75440E-03 (3.74)</td>
<td>8.92592E-03 (3.03)</td>
<td>87.74</td>
</tr>
</tbody>
</table>

*read as 6.19903x10⁻¹ with 0.23% error
Figure 7.16: Depth Dose for electrons with energy distributed between 4.5 and 5 MeV incident on water. Each cell is 0.15 cm thick.

Table 7.8: Depth Dose for 4.5 to 5 MeV electrons incident on water.

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>MCNP (MeV/incident electron)</th>
<th>MMC (MeV/incident electron)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.15</td>
<td>2.91705E-01 (0.19)*</td>
<td>3.34048E-01 (0.21)</td>
<td>14.52</td>
</tr>
<tr>
<td>0.30</td>
<td>3.01231E-01 (0.20)</td>
<td>3.37207E-01 (0.21)</td>
<td>11.94</td>
</tr>
<tr>
<td>0.45</td>
<td>3.10708E-01 (0.20)</td>
<td>3.43172E-01 (0.22)</td>
<td>10.45</td>
</tr>
<tr>
<td>0.60</td>
<td>3.27239E-01 (0.20)</td>
<td>3.46840E-01 (0.22)</td>
<td>5.99</td>
</tr>
<tr>
<td>0.75</td>
<td>3.47705E-01 (0.22)</td>
<td>3.53371E-01 (0.23)</td>
<td>1.63</td>
</tr>
<tr>
<td>0.90</td>
<td>3.73500E-01 (0.24)</td>
<td>3.67055E-01 (0.23)</td>
<td>1.73</td>
</tr>
<tr>
<td>1.05</td>
<td>3.94805E-01 (0.24)</td>
<td>3.84619E-01 (0.24)</td>
<td>2.58</td>
</tr>
<tr>
<td>1.20</td>
<td>4.09459E-01 (0.25)</td>
<td>4.01575E-01 (0.25)</td>
<td>1.93</td>
</tr>
<tr>
<td>1.35</td>
<td>4.11362E-01 (0.26)</td>
<td>4.05738E-01 (0.25)</td>
<td>1.37</td>
</tr>
<tr>
<td>1.50</td>
<td>3.96308E-01 (0.27)</td>
<td>3.87491E-01 (0.27)</td>
<td>2.22</td>
</tr>
<tr>
<td>1.65</td>
<td>3.62249E-01 (0.30)</td>
<td>3.49194E-01 (0.30)</td>
<td>3.60</td>
</tr>
<tr>
<td>1.80</td>
<td>3.07108E-01 (0.34)</td>
<td>2.85157E-01 (0.35)</td>
<td>7.15</td>
</tr>
<tr>
<td>1.95</td>
<td>2.36249E-01 (0.41)</td>
<td>2.02581E-01 (0.45)</td>
<td>14.25</td>
</tr>
<tr>
<td>2.10</td>
<td>1.54440E-01 (0.54)</td>
<td>1.19142E-01 (0.62)</td>
<td>22.86</td>
</tr>
<tr>
<td>2.25</td>
<td>8.21783E-02 (0.77)</td>
<td>5.57388E-02 (0.95)</td>
<td>32.17</td>
</tr>
<tr>
<td>2.40</td>
<td>3.06438E-02 (1.27)</td>
<td>2.13069E-02 (1.56)</td>
<td>30.47</td>
</tr>
<tr>
<td>2.55</td>
<td>6.74965E-03 (2.64)</td>
<td>5.95504E-03 (2.92)</td>
<td>11.77</td>
</tr>
</tbody>
</table>

*read as 2.91705x10^{-1} with 0.19% error
Figure 7.17 shows the ratio of FOM for MMC to MCNP for the depth dose calculations given in Figures 7.13-7.16. A comparison of the computational speed-up can be done by comparing the FOM for the two methods of transport. The ratio of FOM are plotted as a function of tally bin for each of the four incident energy groups. The ratio of FOM range from about 1.5-2.25. This implies that a MMC calculation is about 1.5-2.25 times faster than the corresponding MCNP calculation, depending on the energy and tally of interest. Because the kugels were defined with a diameter equal to 3 times an electron sub-step, the ideal maximum increase in speed is 3.0. Since MCNP is performing many tasks in addition to the actual electron transport this factor of 3.0 will decrease. Furthermore, the sampling of sub-bins for θ and φ slows down the calculation. Using perhaps a logarithmically spaced grid for these distributions could decrease the sampling time while still describing the distribution in enough detail.

![Figure 7.17: Ratio of MMC FOM to MCNP FOM for depth dose calculations.](image-url)
8. Conclusions

MCNP4B was verified against a wide range of electron/photon experiments including high energy bremsstrahlung production and electron transmission and reflection. The bremsstrahlung spectral shape and mean energy compared well across three benchmark experiments. The energy integrated yields agreed within about 10% for cell tallies and 5% for detector tallies when comparing to the experiments of Faddegon et al., except for a few points near 0° and 90°. The cell tally energy integrated yields for O'Dell, however, agreed to within 5% of the experiment, and were slightly higher than the experimental results. The calculations of electron transmission based on the experiments of Ebert et al. compare within 5-15% for silver and uranium, but there are highly significant deviations for carbon. The backscatter verification calculations, for the most part, agree with experiment within 8-20%, with the range of data from several experiment spanning the MCNP results. The overall agreement suggests that electron backscatter calculations in MCNP still warrant improvement.

Several physics parameters have been shown to affect the results and efficiency of the calculations. The choice of bremsstrahlung angular model was shown to impact the calculated results with cell and detector tallies showing better agreement when the same model is used. The electron sub-step artifacts for bremsstrahlung sampling in MCNP4A were shown to be mitigated in MCNP4B. The energy grid sampling scheme was shown to affect the integrated bremsstrahlung yields at high angles, and significantly impacted the results of electron transmission for carbon, but showed a marginal effect for silver and uranium. The bremsstrahlung splitting scheme presently in MCNP could be enhanced by a modified splitting scheme that has undergone preliminary testing. Furthermore, the effect of including knock-on electrons and secondary photons, as well as varying the energy grid and straggling schemes was studied for a suite of depth dose in water calculations.

This study has also demonstrated the significant improvement in the default performance of MCNP4B compared to MCNP4A. Specifically, the enhancements in secondary particle production algorithms and ESTEP performance, as well as improved stopping powers and energy loss parameters have been demonstrated.

The calculations done using the default settings in MCNP4B show excellent overall agreement with experiment. This study has shown that the default parameters should be modified in a few instances. The electron transmission comparisons in carbon show improved agreement with experiment when using the nearest group energy indexing algorithm (DBCN:18=1) option. It is therefore recommended that the DBCN:18=1 be used for high energy electrons (~10 MeV) in low Z materials. Furthermore, after further verification for the full range of experiments and representative target thicknesses in this study, the modified BNUM splitting scheme should be made default in MCNP4C.

There are several areas that can be addressed in further study. The energy indexing algorithms still need to be studied further. The bremsstrahlung angular distributions can be improved, since the energy spectra are already in excellent agreement. More computer time should be invested in the calculations presented here to assess the statistical convergence of the differential energy spectra. Finally, more benchmark studies should be performed to examine a wider range of experiments.

In addition to the verification study, a Macro Monte Carlo (MMC) algorithm has been developed and implemented into MCNP4B. This algorithm makes use of a previously generated electron data library to perform the electron transport. For this study, MCNP was used to generate the
libraries, and the necessary transport information needed in the library for accurate simulations has been determined. The MMC algorithm has been shown to improve the speed of the MCNP calculation by a factor of 1.5-2.25 for a limited range of one-dimensional depth dose in water calculations. The MMC and MCNP calculations show excellent agreement for a range of energies. The agreement between the MMC and MCNP calculation decreases with the incident energy of the electron. Furthermore, as a few groups around the world are developing their own Macro Monte Carlo algorithms and data libraries\textsuperscript{8-11}, these libraries may become available for implementation in MCNP. The algorithms are now in place in MCNP for the code to be able to effectively use this method and associated libraries in electron transport.
9. References


Appendix I: MCNP Verification Input Files

Input File A.1: Faddegon input files

This input file is based on the aluminum with stainless steel configuration. The changes needed for lead and beryllium are indicated in *italics*.

Al Bremsstrahlung Benchmark - Faddegon

- this simulation will be compared with the experimental data
- aluminum target
- 15 MeV beam
- includes stainless steel entrance window
- this run should be used for angle less than 10 degrees

```
c 1 1 -4.51 -1 2 -3  Ti exit window
2 2 -2.338 -4 5 -6  Si current monitor
3 3 -7.9874 -21 20 -3  s.s. exit window
4 4 -2.705 -10 14 -12  Al target
4 4 -11.34 -10 14 -12  Pb target
4 4 -1.848 -10 14 -12  Be target
100 0 -200 -300 301  0 degree
101 0 -201 200 -300 301  1
102 0 -202 201 -300 301  2
103 0 -204 203 -300 301  4
104 0 -206 205 -300 301  10
105 0 -208 207 -300 301  30
106 0 -210 209 -300 301  60
107 0 212 211 -300 301  90
998 0 -999 #4 #100 #101 #102 #103 #104 #105
 #106 #107 #1 #2 #3
999 0 999
```

```
1  pz 2.60  $ exit window
2  pz 2.587
[Pb and Be]
1  pz 3.30  $ exit window
2  pz 3.287
3  cz 1.8
4  pz 2.2  $ current monitor
5  pz 2.19
[Pb and Be]
4  pz 2.9  $ current monitor
5  pz 2.89
6  cz 0.977
10  pz 0.0  $ Al target
12  cz 3.63
14  pz -3.60074
```
[Pb]
10 pz 0.0 $Pb$ target
12 cz 1.5829
14 pz -0.8051

[Be]
10 pz 0.0 $Be$ target
12 cz 3.6364
14 pz -6.3149
20 pz 0.9 stainless steel window
21 pz 0.9051
100 pz 2.601 $surface$ for starting source

[Pb and Be]
100 pz 3.301 $surface$ for starting source

c cones for cell tallies
200 kz 0. 7.6158e-5 -1 $0.5$ degree
201 kz 0. 6.8570e-4 -1 $1.5$
202 kz 0. 1.9063e-3 -1 $2.5$
203 kz 0. 3.7409e-3 -1 $3.5$
204 kz 0. 6.1940e-3 -1 $4.5$
205 kz 0. 2.8004e-2 -1 $9.5$
206 kz 0. 3.4351e-2 -1 $10.5$
207 kz 0. 3.2010e-1 -1 $29.5$
208 kz 0. 3.4697e-1 -1 $30.5$
209 kz 0. 2.8821e0 -1 $59.5$
210 kz 0. 3.1240e0 -1 $60.5$
211 kz 0. 1.3131e4 -1 $89.5$
212 kz 0. 1.3131e4 1 $90.5$

c spheres for cell tallies (1 mm radial thickness)
300 so 300.
301 so 299.9

c outside world

999 so 500

mode p e
imp:p 1 12r 0
imp:e 1 12r 0
cut:p j 0.145 3j
cut:e j 0.145 3j
phys:e 15.8j
sdef par=3 sur=100 pos=0 0 2.601 vec=0 0 -1 dir=1 rad=d1 erg=15.

[Pb and Be]
sdef par=3 sur=100 pos=0 0 3.301 vec=0 0 -1 dir=1 rad=d1 erg=15.
si 1 0.05

c
note: fm tally multipliers convert to per steradian
by multiplying by (300 cm)$^2$
this is the source to detector distance
the energy spectra, to agree with Faddegon, must be
c divided by the width of the energy bin
c
c cell tallies
f4:p 100 6i 107
fm4 9.e4 $ convert to per steradian
fq4 e f
c
c ring detectors
c the first and last tally is offset slightly since detectors
c located right on a surface cause trouble
cf5 0 degree
f5z:p -300.01 0.01 0.
fm5 9e4
cf15 1 degree
f15z:p -299.9543 5.2357 0.
fm15 9e4
cf25 2 degree
f25z:p -299.8172 10.4698 0.
fm25 9e4
cf35 4 degree
f35z:p -299.2692 20.9269 0.
fm35 9e4
cf45 10 degree
f45z:p -295.4423 52.0945 0.
fm45 9e4
cf55 30 degree
f55z:p -259.8076 150. 0.
fm55 9e4
cf65 60 degree
f65z:p -150. 259.8076 0.
fm65 9e4
cf75 90 degree
f75z:p -0.01 300. 0.
fm75 9e4
c mean energy tallies
c cell
*fl4:p 100 6i 107 $ divide by f4 tally to get mean energy
fm14 9.e4
e14 15.
fq14 f e

c detector
cf105 0 degree
*fl105z:p -300.01 0.01 0.
fm105 9e4
e105 15.
fq105 f e
cf115 1 degree
*fl115z:p -299.9543 5.2357 0.
fm115 9e4
e115 15.
fq115 f e
fc125 2 degree
*f125z:p -299.8172 10.4698 0.
fm125 9e4
e125 15.
fq125 f e
fc135 4 degree
*f135z:p -299.2692 20.9269 0.
fm135 9e4
e135 15.
fq135 f e
fc145 10 degree
*f145z:p -295.4423 52.0945 0.
fm145 9e4
e145 15.
fq145 f e
fc155 30 degree
*f155z:p -259.8076 150. 0.
fm155 9e4
e155 15.
fq155 f e
fc165 60 degree
*f165z:p -150.259.8076 0.
fm165 9e4
e165 15.
fq165 f e
fc175 90 degree
*f175z:p -0.01 300. 0.
fm175 9e4
e175 15.
fq175 f e
e0  0.14 0.18 0.22 0.27 0.32 0.38 0.44 0.51 0.58 0.67 0.76
  0.86 0.96 1.08 1.20 1.33 1.47 1.62 1.78 1.95 2.12 2.31
  2.51 2.72 2.94 3.17 3.41 3.66 3.93 4.20 4.49 4.80 5.11
  5.44 5.78 6.13 6.49 6.88 7.27 7.68 8.10 8.54 8.99 9.45
  9.94 10.43 10.94 11.47 12.02 12.58 13.15 13.75 14.35
  14.98 15.63

c titanium
m1  22000 1
c Si
m2  14000 1
c stainless
m3  24000 -18.0 28000 -8.0 26000 -76.0

c aluminum
m4  13027 1
c Pb
m4  82000 1
c Be
m4  4009 1
print
nps 6000000
prdmp 2j 1 1
Input File A.2: Faddegon, Aluminum target, no stainless steel entrance window

This input file is based on the aluminum without stainless steel configuration. The changes needed for lead and beryllium are indicated in italics.

Al Bremsstrahlung Benchmark - Faddegon

c this simulation will be compared with the experimental data
c aluminum target
c 15 MeV beam
c no stainless steel entrance window
c this run should be used for angle greater than 10 degrees

c
1 1 -4.51 -1 2 -3 $ Ti exit window
2 2 -2.338 -4 5 -6 $ Si current monitor
4 4 -2.705 -10 14 -12 $ Al target
4 4 -11.34 -10 14 -12 $ Pb target
4 4 -1.848 -10 14 -12 $ Be target
100 0 -200 -300 301 $ 0 degree
101 0 -201 200 -300 301 $ 1
102 0 -202 201 -300 301 $ 2
103 0 -204 203 -300 301 $ 4
104 0 -206 205 -300 301 $ 10
105 0 -208 207 -300 301 $ 30
106 0 -210 209 -300 301 $ 60
107 0 212 211 -300 301 $ 90
998 0 -999 #4 #100 #101 #102 #103 #104 #105
 #106 #107 #1 #2
999 0 999

1  pz 2.60 $ exit window
2  pz 2.587

[Pb and Be]
1  pz 3.30 $ exit window
2  pz 3.287
3  cz 1.8
4  pz 2.2 $ current monitor
5  pz 2.19

[Pb and Be]
4  pz 2.9 $ current monitor
5  pz 2.89
6  cz 0.977
10 pz 0.0 $ Al target
12 cz 3.63
14 pz -3.60074

[Pb]
10 pz 0.0 $ Pb target
12 cz 1.5829
14 pz -0.80511

[Be]
10 pz 0.0 $ Be target
12 cz 3.6364
14 pz -6.3149

113
100 pz 2.601 $ surface for starting source

[Pb and Be]

100 pz 3.301 $ surface for starting source

c cones for cell tallies
200 kz 0. 7.6158e-5 -1 $ 0.5 degree
201 kz 0. 6.8570e-4 -1 $ 1.5
202 kz 0. 1.9063e-3 -1 $ 2.5
203 kz 0. 3.7409e-3 -1 $ 3.5
204 kz 0. 6.1940e-3 -1 $ 4.5
205 kz 0. 2.8004e-2 -1 $ 9.5
206 kz 0. 3.4351e-2 -1 $ 10.5
207 kz 0. 3.2010e-1 -1 $ 29.5
208 kz 0. 3.4697e-1 -1 $ 30.5
209 kz 0. 2.8821e0 -1 $ 59.5
210 kz 0. 3.1240e0 -1 $ 60.5
211 kz 0. 1.3131e4 -1 $ 89.5
212 kz 0. 1.3131e4 1 $ 90.5

c spheres for cell tallies (1 mm radial thickness)
300 so 300.
301 so 299.9

c outside world
999 so 500

mode p e
imp:p 1 11 r 0
imp:e 1 11 r 0
cut:p j 0.145 3j
cut:e j 0.145 3j
phys:e 15. 8j
sdef par=3 sur=100 pos=0 0 vec=0 0 2.601 vec=0 0 3.301 dir=1 rad=dl erg=15.

sil 0.05

c note: fm tally multipliers convert to per steradian
by multiplying by (300 cm)^2
this is the source to detector distance
the energy spectra, to agree with Faddegon, must be
divided by the width of the energy bin

c cell tallies
f4:p 100 6i 107
fm4 9.e4 $ convert to per steradian
fq4 e f
c
ring detectors
c the first and last tally is offset slightly since detectors
c located right on a surface cause trouble
fc5 0 degree
fs5z:p -300.01 0.01 0.
fm5 9e4
fc15 1 degree
fl5z:p -299.9543 5.2357 0.
fm15 9e4
fc25 2 degree
f25z:p -299.8172 10.4698 0.
f35 9e4
fc35 4 degree
f35z:p -299.2692 20.9269 0.
f35x: -299.2692 20.9269 0.
f45 9e4
fc45 10 degree
f45z:p -295.4423 52.0945 0.
f55 9e4
fc55 30 degree
f55z:p -259.8076 150. 0.
f65 9e4
fc65 60 degree
f65z:p -150. 259.8076 0.
f75 9e4
fc75 90 degree
f75z:p -0.01 300. 0.
f75x: -0.01 300. 0.
e0  0.14 0.18 0.22 0.27 0.32 0.38 0.44 0.51 0.58 0.67 0.76 
    0.86 0.96 1.08 1.20 1.33 1.47 1.62 1.78 1.95 2.12 2.31 
    2.51 2.72 2.94 3.17 3.41 3.66 3.93 4.20 4.49 4.80 5.11 
    5.44 5.78 6.13 6.49 6.88 7.27 7.68 8.10 8.54 8.99 9.45 
    9.94 10.43 10.94 11.47 12.02 12.58 13.15 13.75 14.35 
    14.98 15.63

c titanium
m1 220001

c Si
m2 140001

c aluminum
m4 130271

c Pb
m4 820001

c Be
m4 40091

print
nps 6000000

prdmp 2j 1 l

115
Input File A.3: O'Dell, 10.0 or 20.9 MeV incident electrons

The changes necessary for 20.9 MeV electrons are indicated in *italics*.

Au/W Bremsstrahlung Benchmark - O'Dell
c this simulation will be compared with the experimental data
c Au/W target
c 10 MeV beam
c
1 1 -19.24 -10 14 -12       $ W target
2 2 -19.32 20 -14 -12       $ Au target
100 0 -30 35 -31 32 -33 34   $ 0 degree tally
998 0 -.999 #1 #2 #100
999 0 999
10 pz 0.0
12 cz 2.6
14 pz -0.0254678
20 pz -0.0381489
30 pz -25.6
31 py 1.905
32 py -1.905
[20.9 MeV]
31 py 0.635           $ 0.5 in face of secondary target
32 py -0.635
33 px 0.3175
34 px -0.3175
35 pz -25.7
100 pz 1.0           $ surface for starting source

mode p e
imp:p,e 1 3r 0
these high cutoffs are the same as in experiment
cut:p j 4. 3 j
cut:e j 4. 3 j
c change this card when altering source energy
phys:e 10. 8 j
[20.9] phys:e 20.9 8 j
sdef par=3 sur=100 pos=0 0 1.0 vec=0 0 -1 dir=1 rad=d1 erg=10.
[20.9] sdef par=3 sur=100 pos=0 0 1.0 vec=0 0 -1 dir=1 rad=d1 erg=20.9
s1 0.1

c
note: fm tally multipliers convert to per steradian
c by multiplying by (25.6 cm)^2
c this is the source to detector distance
c
cells
fc4 cell tally - forward direction
f4:p 100
fm4 655.36
f4 e f
c detectors
c use point detector for 0 degrees only as a check
fc5 0 degree
f5:p 0 0 -25.5 0.
fm5 655.36

c
e0  4.0 4.2 4.4 4.6 4.8 5.0 5.2 5.4 5.6 5.8 6.0
   6.2 6.4 6.6 6.8 7.0 7.2 7.4 7.6 7.8 8.0 8.4
   8.8 9.2 9.6 10.
[20.9]
e0  4.0 4.2 4.4 4.6 4.8 5.0 5.2 5.4 5.6 5.8 6.0
   6.2 6.4 6.6 6.8 7.0 7.2 7.4 7.6 7.8 8.0 8.4
   8.8 9.2 9.6 10. 10.4 10.8 12.2 12.6 13.0 13.4
  13.8 14.2 14.6 15.0 15.4 15.8 16.2 16.6 17.0
  17.5 18.0 18.5 19.0 19.5 20.2 20.9

c tungsten
m1 74000 1
c gold
m2 79197 1
print
nps 4000000
prdmp 2j 1 1
Input File A.4: Starfelt and Koch

W Bremsstrahlung Benchmark - Starfelt and Koch

c this simulation will be compared with the experimental data

c W target 5.8 g/cm² thickness

c 9.66 MeV beam

c
1 1 -19.24 -10 14 -12 $ W target
100 0 -200 -300 301 $ 0 degree
104 0 -220 210 -300 301 $ 12
998 0 -999 #1 #100 #104
999 0 999

10 pz 0.0 $ W target
12 cz 2.6
14 pz -0.301455 $ corresponds to a 5.8 g/cm² thickness
100 pz 1.0 $ surface for starting source
200 kz 0. 1.49277e-4 -1 $ 0.7 degree
210 kz 0. 4.13928e-2 -1 $ 11.5
220 kz 0. 4.91485e-2 -1 $ 12.5
c spheres for cell tallies
300 so 120.
301 so 119.7
c outside world
999 so 200

mode p e
imp:p,e 1 3r 0
cut:p j 0.4 3j
cut:e j 0.4 3j

c change this card when altering source energy
phys:e 10. 4j 20 2j 0.05 j
sdef par=3 sur=100 pos=0 0 1.0 vec=0 0 -1 dir=1 rad=d1 erg=9.66
si 1 3

c c note: fm tally multipliers convert to per steradian

c by multiplying by (120 cm)²

c this is the source to detector distance

c
c cells
fc4 cell tallies: 0 and 12 degrees
f4:p 100 104
fm4 1.44e4
fq4 e f
c detectors

c use point detector for 0 degrees
fc5 0 degree
f5:p 0 0 -120.1 0.
fm5 1.44e4
c
c ring detector
fc15 12 degree
f15z:p -117.3777 24.9494 0.
f15 1.44e4
  c
e0  0.4 0.58 0.76 0.94 1.12 1.3 1.48 1.66 1.84 2.02 2.2 2.38 
  2.56 2.74 2.92 3.1 3.28 3.46 3.64 3.82 4.0 4.25 4.5 4.75
  5.0 5.4 5.8 6.2 6.6 7.0 7.5 8.0 8.5 9.0 9.46
  c
  ml 74000 1
  print
  nps 15000000
  prdmp 2j 1 1
Input File A.5: Sample input template for Ebert, transmission and backscatter

This input file is based on silver simulations. The changes needed for carbon and uranium are indicated in italics.

Ebert - 10.2 MeV electrons on 4.85 g/cm² Ag

1 1 -10.48 -1 2 -3
2 0 10 -11 -14
3 0 -12 13 -14
4 0 -999 #1 #2 #3
5 0 999

1 pz 0.0 $ target
change surface 2 to alter thickness
2 pz -0.46279
3 cz 1.0
10 pz -10. $ tally surfaces
11 pz -9.99
12 pz 10.
13 pz 9.99
14 cz 12.
100 pz -11
999 so 100

mode p e
imp:p,e 1 3r 0
phys:e 10.2 8j
sdef par=3 sur=100 pos=0 0 -11. vec=0 0 1 dir=1 rad=d1 erg=10.2
sil 0.3
fc1 backscatter - use first cos bin
f1:e 2
tf1 5j 1 2j
fc31 transmission target face - 2nd bin
f31:e 1
fc41 transmission top - 2nd bin
f41:e 3
c0 0 1
fq0 f c
m1 47000 1
[carbon] m1 6000 1
[uranium] m1 92000 1
print
prdmp 2j 1 1
nps 10000
Input File A.6: Input template for 20 MeV electrons in water

This is a master input file which highlights the parameters that were changed in *italics*.

Energy deposition by 20 MeV electrons in water.

1 1 -1. 100 -105 -300
2 1 -1. 105 -110 -300
3 1 -1. 110 -115 -300
4 1 -1. 115 -120 -300
5 1 -1. 120 -125 -300
6 1 -1. 125 -130 -300
7 1 -1. 130 -135 -300
8 1 -1. 135 -140 -300
9 1 -1. 140 -145 -300
10 1 -1. 145 -150 -300
11 1 -1. 150 -155 -300
12 1 -1. 155 -160 -300
13 1 -1. 160 -165 -300
14 1 -1. 165 -170 -300
15 1 -1. 170 -175 -300
16 1 -1. 175 -180 -300
17 1 -1. 180 -185 -300
18 1 -1. 185 -190 -300
19 1 -1. 190 -195 -300
20 1 -1. 195 -200 -300
21 0 (-100: 200: 300)

100 px 0.0
105 px 0.5
110 px 1.0
115 px 1.5
120 px 2.0
125 px 2.5
130 px 3.0
135 px 3.5
140 px 4.0
145 px 4.5
150 px 5.0
155 px 5.5
160 px 6.0
165 px 6.5
170 px 7.0
175 px 7.5
180 px 8.0
185 px 8.5
190 px 9.0
$\text{Emulate ITS 3. (default=0)}$

$sdef \ par=3 \ pos \ 0. \ 0. \ \ sur=100 \ \ vec \ 1. \ 0. \ 0. \ \ dir=1. \ \ erg=20.$

cut:p \ j \ .189

cut:e \ j \ .189

*f8:e,p 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 t
e8 0 .00000001 20.

fq0 f e

tf8 20
+tf18:e 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 t
c0 0. 1.

f1:p 100 19i 200
f101:e 100 19i 200
*f11:p 100 19i 200
*f111:e 100 19i 200
f2:p 100 19i 200
f102:e 100 19i 200

tf1 5j 1
tf101 5j 1
tf11 5j 1
tf111 5j 1
tf2 5j 1
tf102 5j 1
f4:e 1 18i 20
sd4 1. 19r
tf4 20
*tf14:e 1 18i 20
sd14 1. 19r
tf14 20
m1 1000 2 8000 1

Consider also estep=15

$mode p \ e \ [e]$
Appendix J: Modified BNUM sampling patch

*ident,bnum  
*d,ny.444  
if(nwc.eq.6)then  
   bnum=max(zero,ritm)  
   if(bnum.ne.zero)enum=one/bnum  
endif  
*d,bb.14  

c  
c set up to produce none, one, or more photons.  
el=zero  
npa=1  
nb=1  
c  
do splitting or roulette if bnum biasing is used.  
if(bnum.ne.one)then  
   nb=bnum+rang()  
   if(nb.eq.0)then  
      npa=0  
      nb=1  
   endif  
endif  
wb=wgt  
if(bnum.ne.zero)wb=wgt/bnum  
rb=nb  
c  
prepare to make a photon and save the stack.  
sample the site and get the electron energy for each possible photon  
and record energy loss, el.  
5 npb=npb+1  
*d,bb.21,bb.23  
*i,bb.25  
   wgt=wb  
*d,cor4-1.163  
   if(iphon.ne.0.or.fiml(2).eq.0..or.es.lt.elc(2).or.  
   & npa.eq.0)go to 200  
*d,bb.71,bb.74  
*d,cor4-1.167  
*i,bb.149  
   nb=nb-1  
   if(nb.gt.0)go to 5  
*i,bb.151  
   el=el/rb
Appendix K: MCNP Local Calculation Input File for MMC Library

kugel group 1
1  1 -1.0  -1
2  0 -20  1
3  0  20

1  sz 0.32855  0.32855
20  so 1000

mode e
ml 1000 -0.1119 8000 -0.8881
sdef erg=d1 pos=0 0 -0.0001 dir=1 vec=0 0 1 par=3
sil 18.34  20
spl 0  1
ssw 1
imp:p,e 1 1 0
c0 0 1
f1:e 1 20
*f11:e 1 20
f4:e 1
   nps 110000
phys:e 20. 3j 0 2j 0 j
c cut:e j  .816605E-01
c tme 300
prdm2j -1
print
Appendix L: Surface Source Formatting Code

This program is used to read in the binary surface source file generated by MCNP for a local calculation and print out, in ASCII format, any of the information in the surface source file. To change the output of this code, modify lines 1 and 20.

```fortran
program rswf.f
  character*7 fin
  implicit double precision (a-h, o-z)
  i=1
  iusc=8
  iusr=8
  c write(6,*)' input surface file name '
  c read(5,4)fin
  4 format(a7)
  call getarg(i, fin)
    open(iusc, file=fin, status='old', form='unformatted')
    read(iusc) kod, ver, loddat, idtm, probid, aid, knods
    write(6,*) kod, ver, loddat, idtm, probid, aid, knods
    read(iusc) np1, nrss, nrcd, njsw, niss
    write(6,*) np1, nrss, nrcd, njsw, niss
    read(iusc) niwr, mipts
    write(6,*) niwr, mipts
    do 140 i=1, njsw+niwr+nrss+1
      read(iusr) id
    140 continue
    write(6,*)' phase space '
    do 1 i=1, 100000
      read(iusc) a, b, wgt, erg, tme, x, y, z, u, v
    1    write(6,20) a, erg, x, y, z, u, v
  stop
end
```
Appendix M: Post-Processor Library Generation Code

This code generates the $\theta$, $\phi$, and energy distribution files for one local calculation. These files are concatenated to form the library. To run this code, enter a.out i001, where i001 is the input file containing the local calculation energy group, the file name of the formatted surface source information generated with rswf.f (Appendix D), the $\theta$ distribution file name, energy distribution file name, and $\phi$ distribution file name. An example of an input file for a group one local calculation is:

```
1
file1
an001
en001
phi001
```

/* program = lra.c */
/* stored on cfs in /119238/codes/lra.c */
/* 8/5/97 */
/* creates angle bin boundaries */
/* creates energy pdfs */
/* reads in and manipulates (non-binary) output of rswa.f */
/* modified angle and energy bins */
/* 10 phi bins, but first phi bin is then divided into 20 sub-bins */
/* 20 theta bins, but first phi bin is then divided into 20 sub-bins */
/* each theta bin has a phi distribution */
#include <stdio.h>
#include <math.h>
#define NPS 100000
#define COL 9
#define A_BINS 20
#define E_BINS 2
#define E_GROUP 74
#define EGP 114
#define STR 10
#define PI2 1.5707963
#define PBINS 10
#define FBINS 20
/* there are 74 incident energies that comprise 73 energy groups */
/* the energy pdf includes 114 groups to ensure a CDF that goes to 1 */

void hpsort(void); /* 2-D sorting algorithm */
void ohpsort(double*, int); /* 1-D array sorting algorithm */
double libl[NPS+1][COL]; /* array that is sorted */
main(int argc, char *argv[])
{

int i,r,c,j, k;       /* array counters */
double a,b, erg, x, y, z, u, v;               /* values in wssa output */
double lib[NPS][COL];                       /* array to store wssa output */
double radius;                             /* radius of kugel */
double angle[A_BINS+1], angf[FBINS+1];      /* cos theta bin boundaries */
double w[NPS];                             /* direction w, calculated from u and v */
double e[NPS/A_BINS];                      /* energy values from lib array */
double el[NPS-NPS/A_BINS];
double c2theta, twotheta, theta;

double prob[EGP][E_BINS];                 /* prob. of being in an energy group */
double t85_e[EGP];                        /* energy group values */
double t85_r[E_GROUP-1];                  /* kugel radii for each energy group */
int flag;

double pdf[EGP][E_BINS];                  /* pdf for energies w/in ea angle bin */
double cpdf[EGP][E_BINS];                 /* cumulative pdf */
char e_file[STR], a_file[STR], l_file[STR], pfile[STR]; /* file names */
int pntr;                                /* energy group pointer */
int tpab,tpabf,tppb,tppbf;               /* tracks per angle bin */
float stm, ftm, ctm;                     /* computer time variables */

double sign;
double d, omega[3], check;            /* used in calculating omega, which is the */
                                      /* direction of the electron if it */
                                      /* continued straight out the kugel */
double cphi[NPS],cps[NPS/A_BINS][A_BINS]; /* cos phi values */
char ff[A_BINS][STR];
double ptemp[NPS/A_BINS+1];
double p[NPS/A_BINS][A_BINS],pl[NPS/A_BINS+1];
double pb[PBINS+1][A_BINS],pbf[FBINS+1][A_BINS]; /* bin boundaries */

/* start clock */
stm=clock();

/* initialize array to zero */
for(r=0; r<NPS; r++)
  for(c=0; c<COL; c++)
    lib[r][c]=0;
for(r=0; r<EGP; r++)
  for(c=0; c<E_BINS; c++)
    prob[r][c]=0;

/* input file contains: energy group pointer, surface source file name, */
/* angle bin output file name, energy pdf output file name */
/* accessed as command line argument */
filei=fopen(argv[1], "r");
fscanf(filei, "%d %s %s %s %s", &pntr, l_file, a_file, e_file,pfile);
fclose(filei);

/* read in energy groups and kugel radii from Table 85 data */
/* descending order */
ein=fopen("et", "r");
for(k=0; k<EGP; k++)
    fscanf(ein, "%lf", &t85_e[k]);
for(k=0; k<E_GROUP-1; k++)
    fscanf(ein, "%lf", &t85_r[k]);
fclose(ein);

/* for(k=0; k<EGP; k++)
   printf("%f\n", t85_e[k]);
for(k=0; k<E_GROUP-1; k++)
   printf("%f\n", t85_r[k]) */;

/* determine kugel radius based on incident energy */
radius=t85_r[pntr-1];
printf("%.10f\n", radius);

/* read in output of rswa.f (surface source info) */
filel=fopen(l_file, "r");

/* assign columns of lib array to specified variables */
for(i=0; i<NPS; i++)
{
    fscanf(filel, "%lf %lf %lf %lf %lf %lf %lf %lf %lf", 
            &a, &b,&erg, &x, &y, &z, &u, &v);
    lib[i][0]=a;
    lib[i][1]=erg;
    lib[i][2]=x;
    lib[i][3]=y;
    lib[i][4]=z;
    lib[i][5]=u;
    lib[i][6]=v;
    lib[i][8]=b; /* [7] used later */
}
fclose(filel);

/* calculate cos theta for each track */
for(i=0; i<NPS; i++)
{
    /* cos 2theta = (z-radius)/radius (relative to edge of kugel) */
    c2theta=(lib[i][4]-radius)/radius;
    if(c2theta>PI2)
        sign=-1.0;
    else
        sign=1.0;
    /* half angle formula */
    lib[i][7]=sign*sqrt((c2theta+1)/2.);
}

/* assign columns of lib array to specified variables */
for(i=0; i<NPS; i++)
{
    fscanf(filel, "%lf %lf %lf %lf %lf %lf %lf %lf %lf", 
            &a, &b,&erg, &x, &y, &z, &u, &v);
    lib[i][0]=a;
    lib[i][1]=erg;
    lib[i][2]=x;
    lib[i][3]=y;
    lib[i][4]=z;
    lib[i][5]=u;
    lib[i][6]=v;
    lib[i][8]=b; /* [7] used later */
}
fclose(filel);

/* calculate cos theta for each track */
for(i=0; i<NPS; i++)
{
    /* cos 2theta = (z-radius)/radius (relative to edge of kugel) */
    c2theta=(lib[i][4]-radius)/radius;
    if(c2theta>PI2)
        sign=-1.0;
    else
        sign=1.0;
    /* half angle formula */
    lib[i][7]=sign*sqrt((c2theta+1)/2.);
}
/* copy lib to libl to change array bounds to 1..NPS+1 */
/* hpsort uses array bounds starting with 1, not 0 */
for(i=1; i<=NPS; i++)
    for(k=0; k<8; k++)
        libl[i][k]=lib[i-1][k];

/* sort according to cos theta (ascending order) */
hpsort();

/* copy sorted libl back to lib, with correct array bounds */
/* remainder of program uses array with lower bound of 0 */
for(i=0; i<NPS; i++)
    for(k=0; k<8; k++)
        lib[i][k]=libl[i+1][k]; /* sort according to cos theta (ascending order) */
hpsort();

/* number of tracks per angle bin */

tpab=NPS/A_BINS;
tpabf=tpab/FBINS;
tppb=tpab/PBINS;
tppbf=tppb/FBINS;

/* calculate and store angle bin boundaries */
/* angf are the sub-bins for the first ang bin */
for(i=0; i<A_BINS; i++)
    angle[i]=lib[tpab*i][7];
    angle[A_BINS]=lib[NPS-1][7];
for(j=0; j<FBINS; j++)
    angf[j]=lib[j*tpabf][7];
    angf[FBINS]=lib[tpab][7];

/* write angle bin boundaries to file specified in input file */
filea=fopen(a_file, "w"); /* filea=fopen("a_out", "w"); */
for(j=0; j<FBINS; j++)
    fprintf(filea, "%.10e \n", angf[j]);
for(i=0; i<A_BINS; i++)
    fprintf(filea, "%.10e \n", angle[i]);
fclose(filea);

/* calculate w from each b,u,and v */
for(i=0; i<NPS; i++)
{
    if(lib[i][8]>0.)
        sign=1.0;
    else
        sign=-1.0;
    /* these w values are in the same order as lib, i.e. sorted by cos */
\[ w[i] = \text{sign} \times \sqrt{1 - \text{lib}[i][5] \times \text{lib}[i][5] - \text{lib}[i][6] \times \text{lib}[i][6]}; \]

/* calculate omega, the direction of the electron if it continues in the direction defined by the incident and exit points on kugel */
/* \text{lib}[i][7] is \cos \theta */
for (i = 0; i < NPS; i++)
{
    d = \sqrt{\text{lib}[i][2] \times \text{lib}[i][2] + \text{lib}[i][3] \times \text{lib}[i][3] + \text{lib}[i][4] \times \text{lib}[i][4]};
    for (j = 0; j < 3; j++)
        omega[j] = \text{lib}[i][j+2]/d;
    /* printf("%f %f\n", \text{lib}[i][7], cphi[i]); */
}

/* sort cos phi within each theta angular bin */
/* copy cos phi for present theta bin into temp array, and then sort */
/* \text{cps} is now a 2d array with sorted cos phi values for each theta bin */
for (j = 0; j < A_BINS; j++)
{
    for (i = 1; i <= tpab; i++)
        ptemp[i] = cphi[i-1+j*tpab];
    ohpsort(ptemp, tpab);
    for (i = 0; i < tpab; i++)
        cps[i][j] = ptemp[i+1];
}

/* create phi arrays with some correlation to theta bin */
for (j = 0; j < A_BINS; j++)
{
    for (i = 0; i < tpab; i++)
        p[i][j] = cps[i][j];

    /* form equiprobable bin boundaries for each cos phi array */
    /* set uppermost limit to 1.0 */
    for (i = 0; i < A_BINS; i++)
    {
        for (j = 0; j < PBINS; j++)
            pb[j][i] = p[j*tppb][i];
        pb[PBINS][i] = p[tpab-1][i];
        for (j = 0; j < FBINS; j++)
            pbf[j][i] = p[j*tppbf][i];
        pbf[FBINS][i] = p[tppb][i];
    }

    /* print out cos phi bin boundaries to a file */
    filep = fopen(pfile, "w");
    for (i = 0; i <= FBINS; i++)
    {
        for (j = 0; j < 10; j++)
fprintf(filep, "%9.5f", pbf[i][j]);
fprintf(filep, "\n");
for (j=10; j<20; j++)
    fprintf(filep, "%9.5f", pbf[i][j]);
    fprintf(filep, "\n");
}
for (i=0; i<=PBINS; i++)
{
    for (j=0; j<10; j++)
        fprintf(filep, "%9.5f", pb[i][j]);
        fprintf(filep, "\n");
        for (j=10; j<20; j++)
            fprintf(filep, "%9.5f", pb[i][j]);
            fprintf(filep, "\n");
}
fclose(filep);

/* transfer energy values to two 1-D arrays for further processing */
for (i=0; i<tpab; i++)
e[i]=lib[i][1];
for (i=tpab; i<NPS; i++)
e[i-tpab]=lib[i][1];

/* printf("\n Energy values \n");
for (r=0; r<tpab; r++)
{
    for (c=0; c<N_BINS; c++)
        printf("%f ", e[r][c]);
    printf("\n");
} */

/* find probability of being in an energy group */
/* repeat for both energy distributions */
for (i=0; i<tpab; i++)
{
    flag=0;
    k=1;
    while (!flag)
    {
        if ( (e[i] > t85_e[k]) || (k==115))
            /* k==115 ensures energies below last value on Table 85
                are included */
            { prob[k-1][0]=prob[k-1][0]+1.0;
                flag=1;
            }
else
    k=k+1;
}

for(i=0; i<NPS-tpab; i++)
{
    flag=0;
    k=1;
    while(!flag)
    {
        if( (e1[i] > t85_e[k]) || (k==115))
            /* k==115 ensures energies below last value on Table 85 
               are included */
            
            prob[k-1][l]=prob[k-1][l]+1.0;
            flag=1;
        else
            k=k+1;
    }
}

/* construct energy pdfs for each angle bin */
for(i=0; i<EGP; i++)
{
    pdf[i][0]=(prob[i][0])/tpab;
    pdf[i][1]=(prob[i][1])/((A_BINS-1)*tpab);
}

/* construct cumulative pdfs using previous pdfs */
for(j=0; j<E_BINS; j++)
{
    cpdf[0][j]=pdf[0][j];
    for(i=1; i<EGP; i++)
        cpdf[i][j]=cpdf[i-1][j]+pdf[i][j];
}

/* write energy pdfs to file specified in input file */
filee=fopen(e_file, "w");
/* filee=fopen("e_out", "w"); */
for(i=0; i<EGP; i++)
{
    for(j=0; j<E_BINS; j++)
        fprintf(filee, "%10.6f  ", cpdf[i][j]);
    fprintf(filee, "\n");
}
fclose(filee);
/ * cpu time of program */
        ftm=clock();
        printf("used %f seconds computer time\n", (ftm-stm)/1000000);

    }

/* 1D sorting algorithm heapsort */
void ohpsort(double pt[], int t)
{
    unsigned long i, ir, j, l, k, a;
    double rra;

    l=(t >> 1) +1;
    ir=t;

    for(;;)
    {
        if(l>1)
        {
            a=--l;
            rra=pt[a];
        }
        else
        {
            rra=pt[ir];
            pt[ir]=pt[l];
            if(--ir == 1)
            {
                pt[l]=rra;
                break;
            }
        }
        i=l;
        j=1+l;
        while(j<=ir)
        {
            if(j<ir && pt[j] < pt[j+1]) j++;
            if(rra < pt[j])
            {
                pt[i]=pt[j];
                i=j;
                j <<=1;
            }
            else
                j=ir+1;
        }
        pt[i]=rra;
    }

    /* 2D sorting algorithm heapsort */
void hpsort(void)
{
    unsigned long i, ir, j, l, k, a;
    double rra[8];

    l=(NPS >> 1) +1;
    ir=NPS;

    for(;;)
    {
        if(l>1)
        {
            a=--l;
            for(k=0; k<8; k++)
                rra[k]=libl[a][k];
        }
        else
        {
            for(k=0; k<8; k++)
                rra[k]=libl[ir][k];
            for(k=0; k<8; k++)
                libl[ir][k]=libl[l][k];

            if(--ir == 1)
            {
                for(k=0; k<8; k++)
                    libl[l][k]=rra[k];
                break;
            }
        }
    }
    i=l;
    j=l+1;
    while(j<=ir)
    {
        if(j<ir && libl[j][7] < libl[j+1][7]) j++;
        if(rra[7] < libl[j][7])
        {
            for(k=0; k<8; k++)
                libl[i][k]=libl[j][k];

            i=j;
            j <<=1;
        }
        else
        j=ir+1;
    }
    for(k=0; k<8; k++)
        libl[i][k]=rra[k];
}
### Appendix N: MMC Energy Grid

<table>
<thead>
<tr>
<th>Group</th>
<th>Upper Energy Limit (MeV)</th>
<th>Lower Energy Limit (MeV)</th>
<th>Kugel Radius (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20.0</td>
<td>19.5</td>
<td>0.336375</td>
</tr>
<tr>
<td>2</td>
<td>19.5</td>
<td>19.0</td>
<td>0.329625</td>
</tr>
<tr>
<td>3</td>
<td>19.0</td>
<td>18.5</td>
<td>0.322875</td>
</tr>
<tr>
<td>4</td>
<td>18.5</td>
<td>18.0</td>
<td>0.316100</td>
</tr>
<tr>
<td>5</td>
<td>18.0</td>
<td>17.5</td>
<td>0.309300</td>
</tr>
<tr>
<td>6</td>
<td>17.5</td>
<td>17.0</td>
<td>0.302490</td>
</tr>
<tr>
<td>7</td>
<td>17.0</td>
<td>16.5</td>
<td>0.295500</td>
</tr>
<tr>
<td>8</td>
<td>16.5</td>
<td>16.0</td>
<td>0.288240</td>
</tr>
<tr>
<td>9</td>
<td>16.0</td>
<td>15.5</td>
<td>0.280880</td>
</tr>
<tr>
<td>10</td>
<td>15.5</td>
<td>15.0</td>
<td>0.273510</td>
</tr>
<tr>
<td>11</td>
<td>15.0</td>
<td>14.5</td>
<td>0.266130</td>
</tr>
<tr>
<td>12</td>
<td>14.5</td>
<td>14.0</td>
<td>0.258710</td>
</tr>
<tr>
<td>13</td>
<td>14.0</td>
<td>13.5</td>
<td>0.251190</td>
</tr>
<tr>
<td>14</td>
<td>13.5</td>
<td>13.0</td>
<td>0.243590</td>
</tr>
<tr>
<td>15</td>
<td>13.0</td>
<td>12.5</td>
<td>0.235890</td>
</tr>
<tr>
<td>16</td>
<td>12.5</td>
<td>12.0</td>
<td>0.228090</td>
</tr>
<tr>
<td>17</td>
<td>12.0</td>
<td>11.5</td>
<td>0.220220</td>
</tr>
<tr>
<td>18</td>
<td>11.5</td>
<td>11.0</td>
<td>0.212260</td>
</tr>
<tr>
<td>19</td>
<td>11.0</td>
<td>10.5</td>
<td>0.204210</td>
</tr>
<tr>
<td>20</td>
<td>10.5</td>
<td>10.0</td>
<td>0.196080</td>
</tr>
<tr>
<td>21</td>
<td>10.0</td>
<td>9.5</td>
<td>0.187840</td>
</tr>
<tr>
<td>22</td>
<td>9.5</td>
<td>9.0</td>
<td>0.179500</td>
</tr>
<tr>
<td>23</td>
<td>9.0</td>
<td>8.5</td>
<td>0.171080</td>
</tr>
<tr>
<td>24</td>
<td>8.5</td>
<td>8.0</td>
<td>0.162540</td>
</tr>
<tr>
<td>25</td>
<td>8.0</td>
<td>7.5</td>
<td>0.153890</td>
</tr>
<tr>
<td>26</td>
<td>7.5</td>
<td>7.0</td>
<td>0.145140</td>
</tr>
<tr>
<td>27</td>
<td>7.0</td>
<td>6.5</td>
<td>0.136280</td>
</tr>
<tr>
<td>28</td>
<td>6.5</td>
<td>6.0</td>
<td>0.127280</td>
</tr>
<tr>
<td>29</td>
<td>6.0</td>
<td>5.5</td>
<td>0.118153</td>
</tr>
<tr>
<td>30</td>
<td>5.5</td>
<td>5.0</td>
<td>0.109890</td>
</tr>
<tr>
<td>31</td>
<td>5.0</td>
<td>4.58500000</td>
<td>0.100325</td>
</tr>
<tr>
<td>32</td>
<td>4.58500000</td>
<td>4.20450000</td>
<td>0.092750</td>
</tr>
<tr>
<td>33</td>
<td>4.20450000</td>
<td>3.85550000</td>
<td>0.085725</td>
</tr>
<tr>
<td>34</td>
<td>3.85550000</td>
<td>3.53550000</td>
<td>0.079200</td>
</tr>
<tr>
<td>35</td>
<td>3.53550000</td>
<td>3.24210000</td>
<td>0.073125</td>
</tr>
<tr>
<td>36</td>
<td>3.24210000</td>
<td>2.97300000</td>
<td>0.067500</td>
</tr>
<tr>
<td>37</td>
<td>2.97300000</td>
<td>2.72630000</td>
<td>0.062275</td>
</tr>
<tr>
<td>38</td>
<td>2.72630000</td>
<td>2.50000000</td>
<td>0.057425</td>
</tr>
<tr>
<td>39</td>
<td>2.50000000</td>
<td>2.29250000</td>
<td>0.052925</td>
</tr>
<tr>
<td>40</td>
<td>2.29250000</td>
<td>2.10220000</td>
<td>0.048745</td>
</tr>
<tr>
<td>41</td>
<td>2.10220000</td>
<td>1.92780000</td>
<td>0.0448725</td>
</tr>
<tr>
<td>42</td>
<td>1.92780000</td>
<td>1.76780000</td>
<td>0.0412725</td>
</tr>
<tr>
<td>43</td>
<td>1.76780000</td>
<td>1.62100000</td>
<td>0.0379325</td>
</tr>
<tr>
<td>44</td>
<td>1.62100000</td>
<td>1.48650000</td>
<td>0.0348325</td>
</tr>
<tr>
<td>45</td>
<td>1.48650000</td>
<td>1.36310000</td>
<td>0.0319525</td>
</tr>
<tr>
<td>46</td>
<td>1.36310000</td>
<td>1.25000000</td>
<td>0.0292800</td>
</tr>
<tr>
<td>47</td>
<td>1.25000000</td>
<td>1.14630000</td>
<td>0.0268025</td>
</tr>
<tr>
<td>48</td>
<td>1.14630000</td>
<td>1.05110000</td>
<td>0.0245025</td>
</tr>
<tr>
<td>49</td>
<td>1.05110000</td>
<td>0.96388000</td>
<td>0.0223675</td>
</tr>
<tr>
<td>50</td>
<td>0.96388000</td>
<td>0.88388000</td>
<td>0.0203900</td>
</tr>
<tr>
<td>51</td>
<td>0.88388000</td>
<td>0.81052000</td>
<td>0.0185600</td>
</tr>
<tr>
<td>52</td>
<td>0.81052000</td>
<td>0.74325000</td>
<td>0.0168650</td>
</tr>
<tr>
<td>53</td>
<td>0.74325000</td>
<td>0.68157000</td>
<td>0.0153000</td>
</tr>
<tr>
<td>54</td>
<td>0.68157000</td>
<td>0.62500000</td>
<td>0.0138550</td>
</tr>
<tr>
<td>55</td>
<td>0.62500000</td>
<td>0.57313000</td>
<td>0.0125225</td>
</tr>
<tr>
<td>Group</td>
<td>Upper Energy Limit (MeV)</td>
<td>Lower Energy Limit (MeV)</td>
<td>Kugel Radius (cm)</td>
</tr>
<tr>
<td>-------</td>
<td>--------------------------</td>
<td>--------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>56</td>
<td>0.57313000</td>
<td>0.52556000</td>
<td>1.12975e-2</td>
</tr>
<tr>
<td>57</td>
<td>0.52556000</td>
<td>0.48194000</td>
<td>1.01700e-2</td>
</tr>
<tr>
<td>58</td>
<td>0.48194000</td>
<td>0.44194000</td>
<td>9.13750e-3</td>
</tr>
<tr>
<td>59</td>
<td>0.44194000</td>
<td>0.40526000</td>
<td>8.19500e-3</td>
</tr>
<tr>
<td>60</td>
<td>0.40526000</td>
<td>0.37163000</td>
<td>7.33250e-3</td>
</tr>
<tr>
<td>61</td>
<td>0.37163000</td>
<td>0.34078000</td>
<td>6.54500e-3</td>
</tr>
<tr>
<td>62</td>
<td>0.34078000</td>
<td>0.31250000</td>
<td>5.83000e-3</td>
</tr>
<tr>
<td>63</td>
<td>0.31250000</td>
<td>0.28656000</td>
<td>5.18275e-3</td>
</tr>
<tr>
<td>64</td>
<td>0.28656000</td>
<td>0.26278000</td>
<td>4.59700e-3</td>
</tr>
<tr>
<td>65</td>
<td>0.26278000</td>
<td>0.24097000</td>
<td>4.06800e-3</td>
</tr>
<tr>
<td>66</td>
<td>0.24097000</td>
<td>0.22097000</td>
<td>3.59225e-3</td>
</tr>
<tr>
<td>67</td>
<td>0.22097000</td>
<td>0.20263000</td>
<td>3.16550e-3</td>
</tr>
<tr>
<td>68</td>
<td>0.20263000</td>
<td>0.18581000</td>
<td>2.78400e-3</td>
</tr>
<tr>
<td>69</td>
<td>0.18581000</td>
<td>0.17039000</td>
<td>2.44375e-3</td>
</tr>
<tr>
<td>70</td>
<td>0.17039000</td>
<td>0.15625000</td>
<td>2.14100e-3</td>
</tr>
<tr>
<td>71</td>
<td>0.15625000</td>
<td>0.14328000</td>
<td>1.87250e-3</td>
</tr>
<tr>
<td>72</td>
<td>0.14328000</td>
<td>0.13139000</td>
<td>1.63500e-3</td>
</tr>
<tr>
<td>73</td>
<td>0.13139000</td>
<td>0.12049000</td>
<td>1.42525e-3</td>
</tr>
</tbody>
</table>
Appendix O: MMC Patch to MCNP

The new variables introduced in this path are described in Table G.1. All of the global variables have been stored in the FIXCOM common block.

Table G.1: MMC patch variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameters</td>
<td></td>
</tr>
<tr>
<td>nabins</td>
<td>number of equiprobable exit angle $\theta$ bin boundaries (21)</td>
</tr>
<tr>
<td>nerg</td>
<td>number of incident energies that form the energy grid (73)</td>
</tr>
<tr>
<td>nebins</td>
<td>number of energy distributions (forward and backscatter) for each energy group (2)</td>
</tr>
<tr>
<td>ngrps</td>
<td>number of energies forming grid for energy loss CDFs (114)</td>
</tr>
<tr>
<td>npbc</td>
<td>number of $\phi$ distributions; one for each exit angle bin (20)</td>
</tr>
<tr>
<td>npbr</td>
<td>number of equiprobable scattering angle $\phi$ bin boundaries (11)</td>
</tr>
<tr>
<td>npbrf</td>
<td>number of sub-bin boundaries for both $\theta$ and $\phi$ (21)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Global variables - FIXCOM</td>
<td></td>
</tr>
<tr>
<td>abp(nerg)</td>
<td>absorptions probabilities</td>
</tr>
<tr>
<td>alib(nabins*nnerg)</td>
<td>cos($\theta$) exit angle bin boundaries</td>
</tr>
<tr>
<td>alf(nabins*nnerg)</td>
<td>sub-bins for exit angle</td>
</tr>
<tr>
<td>elib(ngrps*nnerg,nebins)</td>
<td>energy CDFs</td>
</tr>
<tr>
<td>ergg(ngrps)</td>
<td>energy grid values</td>
</tr>
<tr>
<td>rad(nergy)</td>
<td>kugel radii</td>
</tr>
<tr>
<td>cph(npbr*nnerg,npbc)</td>
<td>cos($\phi$) scattering angle bin boundaries</td>
</tr>
<tr>
<td>cphf(npbrf*nnerg,npbc)</td>
<td>sub-bins for scattering angle</td>
</tr>
</tbody>
</table>

Decks XA and EL (subroutines XACT and ELECTR) have been modified to allow MMC transport. Deck RDEK contains the new subroutine RDLIB which reads in the electron data library. The patch is provided with annotations in *italics*.

```*/
  ELECTRON KUGEL PATCH
  */
  V3.1: D.P. Gierga
  */
  MODIFY COMMON
  */
  ADD TO PARAMETERS
  *delete,zc4a.16 <48>
  9 planck=4.135732d-13,slite=299.7925d0,third=one/3.d0,zero=0.,
  + nabins=21,nergy=73,nebins=2,ngrps=114,npbc=20,npbr=11,npbrf=21)
  */
  PUT IN ARRAYS - /fixcom/
```
*ident, cm4bek
*/ 67
*delete, cm4b.2 <85>
    parameter(nfixcm= maxi+3*maxv+ mtop+ mipt*(24+ mxdt+ 7*mdx)+ nsp
    + 66795,
*i, cm4b.8 <104>
    + abp(nerg), alib(nabins*nerg), alf(nabins*nerg),
    + elib(ngrps*nerg, 2), ergg(ngrps), rad(nerg),
    + cph(npbr*nerg, 20), cphf(npbrf*nerg, 20),
*/
-------------------------------------------------------------
desk xa
*/ ADD KUGEL LIBRARY CALL TO XACT
*ident, xaek
*i, xa.13 <16314>
c
c read in kugel library
    if(idum(1).ne.0) call rdlib
*/
*/ -----------------------------------------------------------
desk rdek
*/ READ IN KUGEL LIBRARY
*addfile, xa <16366>
desk rdek
    subroutine rdlib
*call cm

c
these variables set some of the limits for reading in the arrays
    ia=nerg*nabins
    ib=ngrps*nerg
    id=npbrf*nerg
    k=0
    m=0

c
*/ 67
*/
c
read in electron data library for all incident energies
    open(unit=8, file='libt', status='old')
    1 continue
first read in the sub-bins, and then the regular bin boundaries
    do 5 i=1,npbrf
        read(8,*) alf(i+m)
    5 continue
    m=m+npbrf
    do 10 i=1, nabins
        read(8,*) alib(i+k)
    10 continue
    k=k+nabins
    if(k.ne.ia. and .m.ne.id) goto 1

c
c read in energy pdfs
do 20 i=1, ib
   read(8,*) (elib(i,j), j=1, nebins)
20 continue

c   read in energy group structure
do 40 i=1,ngrps
   read(8,*) ergg(i)
40 continue

c   read in kugel radii for each energy group
do 70 i=1,nerg
   read(8,*) rad(i)
70 continue

c   read in absorption probabilities
do 90 i=1,nerg
   read(8,*) abp(i)
90 continue

k=0
m=0
l=1

91 continue

c   read in cos(phi) boundaries
21 x 20 arrays for both the sub-bins and regular bins are listed alternately in the library. Also, the
20 columns in the array are listed over two lines to make it easier to read the library.
do 100 i=1,21
   read(8,*)(cphf(i+k,j),j=1,10)
   read(8,*)(cphf(i+k,j),j=11,20)
100 continue

k=k+21
do 105 i=1,11
   read(8,*) (cph(i+m,j),j=1,10)
   read(8,*) (cph(i+m,j),j=11,20)
105 continue

m=m+11
l=l+1
if(l.ne.74)goto 91

c   close(unit=8)

write to output file
114 write(iuo,'(/5x,a)')'kugel libraries read in'
return
end

*/
*/  --------------------------------------------------------------- deck el
*/ ADD KUGEL FEATURE TO ELECTRON TRANSPORT
*ident, elek
*i, el.4
c  check kugel energy group
if(idum(l).ne.0)then
write a message to output file if energy range is violated
  if(erg.gt.ergg(l).or.erg.1t.ergg(nerg+l))then
call erprnt(1,1,0,0,0,0,0,0,
1 '40henergy outside kugel library boundaries.')
endif
set ig to be energy group
ig=0
do 2 i=l,nerg
  if(erg.gt.ergg(i+l))goto 7
2 continue
7 ig=i

kp is an offset for elib
jp is an offset for alib
nr is an offset for cph
nf is an offset fo cphf

  kp=(ig-l)*ngrps
  jp=(ig-l)*nabins
  nr=(ig-l)*npbr
  nf=(ig-l)*npbrf
  goto 40
endif

c  sample exit angle
*i,el.32 <27293>
  if(idum(l).ne.0)then
    rl=rang()
    k=rl*(nabins-l)+1
  ia is set so the correct cos(\phi) distribution is sampled
    ia=k

c  assign ir,column pointer for correct energy pdf
c  first alib bin is divided into 20 alf sub-bins
c  l=back-scattered, 2=forward scattered
  if(k.eq.1)then
    ir=1
    rl=rang()
    kf=rl*(npbrf-1)+1
    dn=alf(kf+nf)
  else
    ir=2
    dn=alib(k+jp)
  up=alib(k+jp+1)
endif

c
sample cos(\theta) randomly between bin boundaries
r2=rang()
c\[ct=dn+r2*(up-dn)\]c
scattered the electron
clectron takes step in new direction vectors
uold(1)=uuu
uold(2)=vvv
uold(3)=www

rotas performs a geometry transformation to get the directions in the global reference frame

call rotas(ct,uold,uuu,lev,irt)
c get kugel radius rd
rd=rad(ig)
c calculate distance traveled in kugel
zl=2*rd*ct
pmf=z1
goto 55
dendif

c\*delete,el.36  
55 if(mbd(lmbd+icl).ne.O.or.jsu.ne.O)go to 60
*i,el.61  
c skip directly to energy loss if kugel transport
if(idum(1).ne.0)goto 95
c
*i,el4b.29  
c check for boundary crossing and sample absorption probability
if absorbed, treat like falling below cutoff
if not absorbed, then sample new energy and continue
if(idum(1).ne.0)then
if(pmf.gt.dls)then
sc=dls/(2.*rd)
else
sc=zl/(2.*rd)
endif
r3=rang()
if(r3.lt.sc*abp(ig))goto 170
c sample new energy and group
c save last energy group for in-group scattering test
ip=ig
c a provides a bias in energy CDF
a attempts to bias the CDF to account for where the incident energy is in relation to the group boundaries
rn=rang()
a=(elib(ig+kp,ir))
+ *(ergg(ig)-erg)/(ergg(ig)-ergg(ig+1))
do 96 k=ig,ngrps
   if(rn.lt.(elib(k+kp,ir)-a)/(l-a))goto 97
96 continue
   write(iuo,*)'warning: energy group problem'
   return
97 ig=k
  c
  c sample new energy (energies are in descending order)
  c if statement ensures no negative energy loss
  If the new energy group was sampled to be the same as the old one, it would be possible to sample
  a new energy greater than the old energy, since the energy is sampled randomly within the group.
The old energy is therefore used as an upper bound within the group.

  if(ig.eq.ip)then
    up=eg0
  else
    up=ergg(ig)
  endif
  dn=ergg(ig+1)
  rn=rang()
  en=dn+rn*(up-dn)
  erg=eg0-(d/pmf)*(eg0-en)
  c update pointers and possibly energy group
  c energy group may have changed due to small d/pmf
  for some boundary crossings, the scaling could alter the energy group
  i=ig
  98 if(erg.gt.ergg(i))then
    i=i-1
  goto 98
  else
    ig=i
    kp=(ig-1)*ngrps
    jp=(ig-1)*nabins
  endif
  if(erg.lt.elc(3))goto 170
  goto 139
  endif
  c
  *i,el.103 <27380>
  139 if(idum(l).ne.0)then
     call uplpos(xxx,uuu,lev,d,vel,1)
  goto 141
  endif
  *delete,el.108 <27382>
  141 if(d.eq.dtc)go to 160
  *i,el.110
  if(idum(l).ne.0)then
    c sample cos(phi), the scattering angle at the end of kugel step
    r=rang()
n = r * (npbr - 1) + 1
r1 = rang()

if n equals 1, then sample from the sub-bins in cphf
if (n .eq. 1) then
  r2 = rang()
  n2 = (r2 * (npbrf - 1) + 1)
  cp = cphf(n2 + nf, ia) + r1 * (cphf(n2 + 1 + nf, ia) -
  cphf(n2 + nf, ia))
else
  cp = cph(n + nr, ia) + r1 * (cph(n + 1 + nr, ia) - cph(n + nr, ia))
endif

scale cos(\phi) for boundary crossings
if (pmf .gt. dls) then
  if (cp .ge. 0) cp = cp ** ((dls / pmf))
  if (cp .lt. 0) cp = -(abs(cp) ** ((pmf / dls)))
endif

145 continue
uold(1) = uuu
uold(2) = vvv
uold(3) = www
call rotas(cp, uold, uuu, lev, irt)
c
update pointers
nr = (ig - 1) * npbr
nf = (ig - 1) * npbrf
endif

* <27399>
i, el.123
  if (idum(1) .ne. 0) goto 150
* <27404>
i, el4b.44
  if (idum(1) .ne. 0) goto 40
* <27429>
i, el.132
  if (idum(1) .ne. 0) goto 40
*/
*/ --------------------------------------------------------------
Appendix P: Sample input file for MMC comparisons with MCNP

This file is used to generate the data given in Figure 7.13. To run without the MMC (kugel) option, delete the IDUM card.

Energy deposition by 20 MeV electrons in water - kugels

<table>
<thead>
<tr>
<th>Energy Level</th>
<th>IDUM Card</th>
<th>Energy Deposition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>-100 -105 -300</td>
</tr>
<tr>
<td>2</td>
<td>-1</td>
<td>-105 -110 -300</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>-110 -115 -300</td>
</tr>
<tr>
<td>4</td>
<td>-1</td>
<td>-115 -120 -300</td>
</tr>
<tr>
<td>5</td>
<td>-1</td>
<td>-120 -125 -300</td>
</tr>
<tr>
<td>6</td>
<td>-1</td>
<td>-125 -130 -300</td>
</tr>
<tr>
<td>7</td>
<td>-1</td>
<td>-130 -135 -300</td>
</tr>
<tr>
<td>8</td>
<td>-1</td>
<td>-135 -140 -300</td>
</tr>
<tr>
<td>9</td>
<td>-1</td>
<td>-140 -145 -300</td>
</tr>
<tr>
<td>10</td>
<td>-1</td>
<td>-145 -150 -300</td>
</tr>
<tr>
<td>11</td>
<td>-1</td>
<td>-150 -155 -300</td>
</tr>
<tr>
<td>12</td>
<td>-1</td>
<td>-155 -160 -300</td>
</tr>
<tr>
<td>13</td>
<td>-1</td>
<td>-160 -165 -300</td>
</tr>
<tr>
<td>14</td>
<td>-1</td>
<td>-165 -170 -300</td>
</tr>
<tr>
<td>15</td>
<td>-1</td>
<td>-170 -175 -300</td>
</tr>
<tr>
<td>16</td>
<td>-1</td>
<td>-175 -180 -300</td>
</tr>
<tr>
<td>17</td>
<td>-1</td>
<td>-180 -185 -300</td>
</tr>
<tr>
<td>18</td>
<td>-1</td>
<td>-185 -190 -300</td>
</tr>
<tr>
<td>19</td>
<td>-1</td>
<td>-190 -195 -300</td>
</tr>
<tr>
<td>20</td>
<td>-1</td>
<td>-195 -200 -300</td>
</tr>
<tr>
<td>21</td>
<td>0</td>
<td>(-100 : 200 : 300)</td>
</tr>
</tbody>
</table>

100 px 0.0
105 px 0.5
110 px 1.0
115 px 1.5
120 px 2.0
125 px 2.5
130 px 3.0
135 px 3.5
140 px 4.0
145 px 4.5
150 px 5.0
155 px 5.5
160 px 6.0
165 px 6.5
170 px 7.0
175 px 7.5
180 px 8.0
185 px 8.5
190 px 9.0
195 px 9.5
200 px 10.0
300 so 100.

idum 1
phys:e 20. j 0 j 0 2j 0 j
sdef par=3 pos 0. 0. 0. sur=100 vec 1. 0. 0. dir=1. erg=d1
sil 19.5 20.0
spl 0 1
cut:p j 0.189
cut:e j 0.189
*f8:e 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
*e0 0.00000001 20.
fq0 f e
*f18:e 2
*f28:e 3
*f38:e 4
*f48:e 5
*f58:e 6
*f68:e 7
*f78:e 8
*f88:e 9
*f98:e 10
*f108:e 11
*f128:e 12
*f138:e 13
*f148:e 14
*f158:e 15
*f168:e 16
*f178:e 17
*f188:e 18
*f198:e 19
*f208:e 20
ml 1000 2 8000 1
mode e
imp:e 1 19r 0
imp:p 1 19r 0
nps 100000
print
prdmp 2j 1 1