Simulated Liquid Argon Interactions with Neutrons

by

Kathleen M. Harrington

Submitted to the Department of Physics in partial fulfillment of the requirements for the degree of Bachelor of Science in Physics

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

June 2012

© Kathleen M. Harrington, MMXII. All rights reserved.

The author hereby grants to MIT permission to reproduce and distribute publicly paper and electronic copies of this thesis document in whole or in part.

Author

Department of Physics

May 11, 2012

Certified by

Joseph A. Formaggio
Associate Professor of Physics
Thesis Supervisor

Certified by

Kimberly J. Palladino
Senior Postdoctoral Associate
Thesis Supervisor

Accepted by

Nergis Mavalvala
Undergraduate Thesis Coordinator
Simulated Liquid Argon Interactions with Neutrons

by

Kathleen M. Harrington

Submitted to the Department of Physics
on May 11, 2012, in partial fulfillment of the
requirements for the degree of
Bachelor of Science in Physics

Abstract

The GEANT4 physics simulation program is known to have errors in how hadronic interactions are implemented. This has the potential to cause errors in the Monte Carlos used to determine the expected neutron backgrounds in the MiniCLEAN single phase liquid argon WIMP detector. Elastic and inelastic collisions between neutrons and argon nuclei as well as neutron captures were simulated independently in order to characterize the accuracy of the implementation by GEANT4.9.3.p01 and GEANT4.9.5. The effective cross sections, angular distributions, photons, decay schemes, energy conservation, and momentum conservation were determined through analysis of the neutron tracks created by GEANT4. A large proportion of the interactions behave as expected, however energy and momentum are not conserved by varying degrees of severity with some GEANT4.9.3.p01 inelastic collisions resulting in over twice the correct amount of energy.

Thesis Supervisor: Joseph A. Formaggio
Title: Associate Professor of Physics

Thesis Supervisor: Kimberly J. Palladino
Title: Senior Postdoctoral Associate
Acknowledgments

This thesis would not have been possible without Dr. Kimberly Palladino. I am extremely grateful to you for your guidance and support throughout my work on this project and in working toward graduate school. Your advice and assistance has been invaluable.

I would also like to thank, Dr. Stanley Seibert and the members of the Mini-CLEAN collaboration who helped us rebuild RAT every time GEANT4 decided to update.

Another thank you goes to Professor J. David Litser and Dr. Sean Robinson for all the advice they have given me and for letting me play around with radio telescopes when I should have been working on this thesis.

I am truly indebted and thankful to my parents for the sacrifices they made while helping me achieve what I have, their constant support is something I could not have done without.

Also, thank you Tetazoo for the title to my thesis and a million found memories.
Contents

1 Evidence and Predictions for Dark Matter 17
   1.1 Astrophysics Evidence ............................................. 17
   1.2 Particle Physics Predictions ..................................... 19
   1.3 Direct Detection of Dark Matter .................................. 20

2 Neutron Physics 25
   2.1 Cross Sections ..................................................... 25
   2.2 Cross Section Measurements ...................................... 28
   2.3 Cross Section Databases .......................................... 30
   2.4 Elastic Collisions and Angular Distributions ................. 33

3 Simulations 37
   3.1 Simulation Software ............................................... 37
   3.2 Argon Sheet Simulations .......................................... 38
      3.2.1 Elastic Collisions .......................................... 38
      3.2.2 Inelastic Collisions ........................................ 39
      3.2.3 Neutron Capture .............................................. 39

4 Elastic Collisions 41
   4.1 Elastic Cross Section ............................................. 41
   4.2 Angular Distribution .............................................. 42
   4.3 Energy and Momentum Conservation ............................... 44
   4.4 Summary ............................................................ 48
5 Inelastic Collisions

5.1 Total Inelastic Cross Section ................................................. 49
5.2 Inelastic Final States ............................................................. 50
  5.2.1 Cross Sections of Final States ........................................... 51
  5.2.2 Angular Distribution ....................................................... 53
5.3 Excited States and Gamma Rays ............................................. 55
5.4 Energy and Momentum Conservation ...................................... 60
5.5 Summary ............................................................................. 67

6 Neutron Capture

6.1 Cross Section ........................................................................ 69
6.2 Capture Gammas .................................................................... 70
6.3 Argon 41 Decay ..................................................................... 72
6.4 Summary ............................................................................. 73

7 Conclusions ........................................................................... 75
List of Figures

1-1 The currently known composition of the universe. Dark matter makes up about 23% of the total matter in the universe.[18] ............................................. 18

1-2 The bullet cluster which illustrates the collisionless properties of dark matter. Hot gas from the two galaxies is shaded pink while the dark matter, seen through gravitational lensing, is shaded blue. The hot gas from each galaxy interacted as the galaxies collided but the dark matter pass through undisturbed.[19] ................................................. 19

1-3 Spin-independent elastic WIMP-nucleon cross-section $\sigma$ as function of WIMP mass $m_X$. The new XENON100 limit at 90% CL is shown as the thick (blue) line together with the expected sensitivity (yellow/green band). The limits from XENON100 (2010), EDELWEISS (2011), CDMS (2009), CDMS (2011) and XENON10 (2011) are also shown. Expectations from CMSSM are indicated at 68% and 95% CL (shaded gray, gray contour), as well as the 90% CL areas favored by CoGeNT and DAMA (no channeling) Figure from [3]. ................................................. 21

1-4 Diagram of the processes leading to primary scintillation (S1) light in a liquid noble detector (here Xe), and to secondary (S2) light proportional to the amount of ionization. Recoils dissipate energy as atomic motion, excitation, and ionization. Both excitation and ionization result in excited dimers, $Xe_2$, in either a longer-lived triplet state or a shorter-lived singlet. Figure from [21] ................................................. 22

1-5 A graphic depicting the MiniCLEAN detector which has a the spherical inner vessel completely surrounded by PMTs. ................................. 24
A log-log total neutron argon-40 cross section as measured by Winters et. al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. The difference between the ENDF/B-VII.1 total and ENDF/B-VII.1 elastic at low energy is due to the neutron capture cross section. The significant difference between the ENDF/B-VII.1 inelastic and G4NDL4.0 inelastic is due to G4NDL4.0 including the (n,2n) and (n,3n) final states while ENDF/B-VII.1 does not. ENDF/B-VII.1 total includes elastic, inelastic, capture, (n,2n), and (n,3n).

A linear plot of the total neutron argon-40 cross section as measured by Winters et. al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. The significant difference between the ENDF/B-VII.1 inelastic and G4NDL4.0 inelastic is due to G4NDL4.0 including the (n,2n) and (n,3n) final states while ENDF/B-VII.1 does not. ENDF/B-VII.1 total includes elastic, inelastic, capture, (n,2n), and (n,3n).

A section of resonances of the total neutron argon-40 cross section as measured by Winters et. al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. Argon-40 has a large resonance at about 50 keV which, while partially mitigated by the presence of argon-36, was not detected by the Winters et. al. experiment.

ENDF/B-VII.0 cross sections for the different final states of an inelastic collision between a neutron and an argon nucleus. Only the first six of the 25 (n,n_k) states are shown in this plot. The plot also indicates that ENDF/B-VII does not include the (n,2n) and (n,3n) states in its total inelastic cross section.

G4NDL4.0 cross sections for the different final states of an inelastic collision between a neutron and an argon nucleus. Only the first six of the 23 (n,n_k) states are shown. G4NDL4.0 does not include data for the (n,^3He) final state.
4-1 The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 0.2 and 22 MeV in 0.2 MeV intervals. The simulations implementing GEANT4.9.3 match the G4NDL3.13 data and the simulations implementing GEANT4.9.5 match the G4NDL4.0 data. G4NDL3.13 only includes resonances up to 1 MeV while G4NDL4.0 and ENDF/B-VII includes resonances up to 5 MeV.

4-2 The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 40 and 60 keV in 0.5 keV intervals.

4-3 The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 80 and 110 keV in 0.5 keV intervals.

4-4 The angular distribution of the outgoing neutron during an elastic collision between an argon nucleus and a neutron with 8 MeV of energy. The plots are normalized to one event. The ENDF/B-VII and G4NDL distributions were built from their Legendre coefficients. The simulations match the respective versions of G4NDL and G4NDL4.0 is more similar to ENDF/B-VII.

4-5 The nuclear recoil energy deposited by the initial 5.0 MeV neutron during the elastic collision. The blue markers indicate the energy information in the simulation and the black markers indicate the recoil energy calculated from the simulated scattering angle. The initial neutrons had 5 MeV of kinetic energy. The plots are normalized to one event.

4-6 (a) and (b) are the change in energy for 8.0 MeV neutron simulations in GEANT4.9.3.p01 and GEANT4.9.5. (c) and (d) are the change in energy versus the cosine of the scattering angle which is a linear relationship for some unknown reason. The plots are normalized to one event. The width of the distribution increases in GEANT4.9.5 but the shape remains the same.
4-7 (a) and (b) are the magnitude of the change in momentum vector for the 8.0 MeV neutron simulations in GEANT4.9.3.p01 and GEANT4.9.5. (c) and (d) represent the direction of the change in momentum vector which is nearly isotropic. The plots are normalized to one event.

4-8 The change in momentum versus the change in energy for the 8 MeV simulations from GEANT4.9.3.p01 and GEANT4.9.5. The plots are normalized to one event.

5-1 The total inelastic cross section of argon-40 found in the RAT simulations compared to the well accepted values from ENDF/B-VII.1 and G4NDL3.13 or G4NDL4.0. The (n,2n) and (n,3n) states of ENDF/B-VII.1 are added to the (n,inelastic) values because ENDF/B-VII.1 does not include these states in the total cross section.

5-2 The cross section of the final states (n,2n) and (n,α) for GEANT4.9.3.p01 and GEANT4.9.5. The simulations lie along G4NDL3.13 or G4NDL4.0 while G4NDL4.0 matches ENDF/B-VII.1.

5-3 The angular distribution of the neutron in the inelastic collision in the GEANT4.9.5. The angular distribution is isotropic for all final states except the (n,nk) states. (a) is the (n,n₁) final state for 7.0 MeV neutrons which is non-isotropic and has a distribution that depends on the initial energy of the neutron and (b) is the (n,2n) final state which is expected to be isotropic. The plots are normalized to one event.

5-4 The total energy of the gamma rays released during an inelastic collision with a initial neutron energy of 3.8 MeV or 7.0 MeV. The total gamma energy represents the final energy state of the argon-40 nucleus. The GEANT4.9.3.p01 states are extremely non-physical. The expected energy levels are listed in Table 5.2.

5-5 The simulated cross sections of the first five excited states of the argon-40 nucleus for the GEANT4.9.5 simulations.
5-6  Gamma rays released during the deexcitation of argon-40 excited by an inelastic collision with a 4.0 MeV neutron. (a) and (b) show the entire spectrum while (c) and (d) are semi-log plots of (a) and (b). The expected energies of the expected gamma rays are listed in Table 5.2. (e) and (f) are zoomed to show gammas with energy less than 5 keV. All plots are normalized to one event.

5-7  The change in energy for the (n,nk) states from the 3.0 MeV and 5.0 MeV simulations using GEANT4.9.3.p01 and GEANT4.9.5. All plots are normalized to one event.

5-8  The change in the kinetic energy of the initial neutron for the (n,nk) states in the 10 MeV neutron simulations. The larger (more negative) changes in energy are due to inelastic scattering while the smaller changes are caused by quasi-elastic scattering. Both plots are normalized to one event.

5-9  The magnitude of the change in momentum for the 9.0 MeV neutron simulations. Both plots are normalized to one event.

5-10 The correlations between number and energy of the small gammas, the change in energy, and the change in momentum for the (n,nk) final states only of the 5.0 MeV GEANT4.9.3.p01 neutron simulation. The number, (a), and energy, (b), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in energy for the collision. The number, (c), and energy, (d), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in momentum for the collision. (e) is the change in energy of the collision compared to the change in momentum of the collision.
5-11 The correlations between number and energy of the small gammas, the change in energy, and the change in momentum for the \((n, n_k)\) final states only of the 5.0 MeV GEANT4.9.5 neutron simulation. The number, \((a)\), and energy, \((b)\), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in energy for the collision. The number, \((c)\), and energy, \((d)\), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in momentum for the collision. \((e)\) is the change in energy of the collision compared to the change in momentum of the collision.

6-1 The simulated cross section for neutron capture compared to ENDF/B-VII.1 and G4NDL3.13 or G4NDL4.0. Errors on the data points are from simulation statistics.

6-2 The simulation cross section for neutron capture zoomed in on a sharp resonance and a softer resonance. The simulation cross section matches with the datasets from ENDF/B-VII.1 and G4NDL4.0. Errors on the data points are from simulation statistics.

6-3 The individual gamma rays released on capture of a 1e-4 eV neutron compared to the expected spectrum from ENSDF. The spectrum from the simulation does not match the spectrum from ENSDF; the simulation has extra lines and is missing some from ENSDF.
List of Tables

5.1 The unique decay products created during inelastic scatters. These were used to determine what type of inelastic scatter had occurred. 51

5.2 The energy levels of argon-40 as listed in ENSDF and G4NDL4.0, as well as the gammas released during de-excitation and their branching ratios. All energies in keV. The different gamma energies in the fifth excited state, 1087.6keV and 682.9keV, are different transitions to the second and third state respectively. 57

5.3 The ratios of all gammas created in the GEANT4.9.5 simulations with energies less that 3.6 MeV. All energies in keV and all errors are from statistics of simulation 58
Chapter 1

Evidence and Predictions for Dark Matter

Dark matter is an over 80 year old problem in the field of physics. Indications of dark matter, originally thought to be conventional non-radiating matter, were first found in astronomical observations in the 1933. Since that time, there have been many theories regarding the form of dark matter and the presence of dark matter has become vitally important to several well accepted theories in physics. In this chapter I will summarize the current state of knowledge about dark matter and the ongoing attempts to detect it.

1.1 Astrophysics Evidence

The first hints of dark matter were found by Zwicky when he measured the velocities of nearby galaxy clusters and found they were behaving as though there was large amounts of undetectable matter present[23]. A few decades later, the measurements of galactic rotation curves indicated the presence of significant amounts of undetectable matter on galactic scales[17]. Originally dark matter was simply thought to be matter which was non-luminous and therefore extremely difficult to detect using the available technology. Further experiments have made the theory of dark matter much more complex than initially believed.
Figure 1-1: The currently known composition of the universe. Dark matter makes up about 23% of the total matter in the universe.[18]

The total amount of dark matter in the universe is known through several measured cosmological parameters. The universe was found to be flat using precise measurements in the Hubble parameter and angular fluctuations in the cosmic microwave background[14]. A flat universe means there is exactly enough matter for space to be Euclidean and that the ratio of the density of the universe to the critical density equals one. Even though the CMB indicates the universe is flat, the amount of light and matter visible does not make up enough mass to account for this flatness, implying there is some amount of invisible matter in the universe. Experiments have since determined this undetected mass is a combination of dark matter and dark energy, differentiated by how each affects the evolution of the universe, and that dark matter consists of approximately 23% of the matter in the universe[18].

In addition to the amount of dark matter, it has been found that dark matter does not fully consist of baryons[15]. Baryons are particles which consist of three quarks such as protons and neutrons. Measurements of baryon acoustic oscillations in the cosmic microwave background give the density of baryons in the universe to be $4.6 \pm 0.1\%$ of the universe. This leaves $22 \pm 2\%$ of matter in the universe as non-baryonic dark matter[9].

Many other experiments have shown that dark matter is also believed to be cold and collisionless. Dark matter has been found to be essential to the evolution of the universe, especially in the formation of structure in the universe. N-body simulations have shown that only cold (non-relativistic) dark matter leads to the formation of
structures of resembling those found in the universe today[12]. The discovery of
dark matter halos around galaxies implies that dark matter must be collisionless
meaning dark matter must have an extremely small collision cross section[15]. The
best proof that dark matter is collisionless are clusters such as the bullet cluster
(Figure 1-2), where two galaxies have collided. In Figure 1-2, the hot gas from the
two galaxies imaged in the x-ray is shaded in pink while the dark matter detected
through gravitational lensing is in blue. The hot gas was slowed as the galaxies passed
through each other while the dark matter did not interact through the collision. The
dark matter must be collisionless for it to not interact to such an extent.

1.2 Particle Physics Predictions

In addition to the significant evidence for dark matter gathered in astrophysics, par-
ticle physics has many predictions which could explain the existence of dark matter
and its possible make-up. There are a large numbers of theories describing possible
candidates for dark matter which more or less account for the observed properties of
dark matter, any one of these theories could be correct or it could be a combination of these theories[18].

One of the more accepted theories is that dark matter consists of Weakly Interacting Massive Particles (WIMPs). WIMPs are any particle which interacts through the weak force, but not the electromagnetic force, and has a mass larger than the known particles; several candidates for WIMPs are predicted from Supersymmetry, an extension of the Standard Model of particle physics. Supersymmetry is an unproven but favored extension to the Standard Model because it solves the hierarchy problem and enables grand unification[12]. In Supersymmetry, each of the particles in the Standard Model has a supersymmetric partner. The lightest supersymmetric particle (LSP) is stable over the time-scale of the universe and could have all the necessary properties to be a WIMP[12].

Another compelling reason for WIMPs to be dark matter is the “WIMP miracle,” which predicts that weakly interacting particles should be created in the observed amounts during the big bang. The WIMP miracle occurs due to the combined affects of weak interactions and an expanding universe. Initially the temperature of the universe is above the mass of the particle and the WIMPs are created and annihilated at equal rates. As the universe expands the temperature drops and the WIMPs annihilate more often than they are created. In thermal equilibrium all the WIMPs would be annihilated and would not be present in the universe today, however this can be avoided if the particles “freeze out” of thermal equilibrium. This occurs if the expansion of the universe separates the particles by large enough distances that they cease to interact with each other[12]. The parameters of the WIMP freeze out necessary to obtain todays dark matter densities and the estimated values from supersymmetry imply a WIMP with a mass on the order of $100 \text{ GeV}/c^2[21]$.

1.3 Direct Detection of Dark Matter

There are three main avenues for detecting dark matter: after it is produced in an accelerator, indirectly from annihilation around massive astrophysical objects, and
Figure 1-3: Spin-independent elastic WIMP-nucleon cross-section $\sigma$ as function of WIMP mass $m_\chi$. The new XENON100 limit at 90% CL is shown as the thick (blue) line together with the expected sensitivity (yellow/green band). The limits from XENON100 (2010), EDELWEISS (2011), CDMS (2009), CDMS (2011) and XENON10 (2011) are also shown. Expectations from CMSSM are indicated at 68% and 95% CL (shaded gray, gray contour), as well as the 90% CL areas favored by CoGeNT and DAMA (no channeling) Figure from [3].
directly through nuclear scattering in detectors. No dark matter signatures have been detected in accelerators nor has there been any conclusive detection from astronomical observation[21]. Currently, direct detection of dark matter offers the best chance of a detection and many different attempts to directly detect the various predicted types of dark matter are underway[21]. Here I will limit the discussion of direct detection to the methods used to detect WIMPs. Direct detection of WIMPs involves detecting a nuclear recoil which can be shown to be from a WIMP particle colliding with the nucleus. There have been a few claimed detections, however these are inconclusive because there has not been any repeated measurements at the same values[3, 20, 1, 2]. Figure 1-3 shows WIMP cross section versus WIMP mass with exclusion limits from XENON100, EDELWEISS, CDMS, and XENON10 along with claimed detections from DAMA and CoGeNT and predictions from CMSSM[3].
Liquid Noble detectors such as MiniCLEAN and XENON100 employ one of them many of direct detection methods currently used in the search for dark matter. MiniCLEAN will use liquid Argon while XENON100 uses liquid Xenon. Liquid noble detectors are desirable because they are easier to scale to large sizes, a useful property when the expected detection rate is less than 1 event per 10 kg of target material[21]. Figure 1-4 depicts scintillation in liquid xenon following recoils. A WIMP collision causes a nuclear recoil which leads to both excitation and ionization. The excitation and ionization lead to excited dimers which then scintillate and release of photon of wavelength 175nm for Xenon or 128nm for Argon. The excited dimer can be in either a singlet state or a triplet state, where the triplet state has a longer lifetime. Nuclear recoils produce more singlet state dimers, allowing discrimination between nuclear and electronic recoils based on the detected pulse shape[21]. It is also possible to detect the electrons released during the ionization caused by the nuclear recoil. Most of the current dark matter experiments detect either the scintillation light, the ionization electrons, or a combination of the two[21].

Figure 1-5 shows the design of the MiniCLEAN experiment which is a single phase liquid Argon detector. A sphere of liquid Argon is surrounded by 92 PMTs which allow for spacial reconstruction of the detected collision and the entire experiment will be surrounded by a an instrumented water shield and placed deep underground. The water veto, placement underground, spacial reconstruction, and scintillation light timing are all used to decrease the expected neutron background. Because neutrons interact with nuclei via the weak force, a collision between a neutron and an argon nucleus looks extremely similar to a collision between a WIMP and an argon nucleus if the neutron only collides once in the detector. Neutrons are expected to come from the muon spallation in the surrounding rock and alphas from fissions of Uranium and Thorium interacting with the experimental apparatus. Placing the detector underground significantly reduces neutrons produced due to cosmic rays and the water veto will stop lower energy neutrons produced outside the experimental apparatus.

The hardest neutron source to account for is the experimental apparatus, for example alpha particles interacting with the Boron in the PMT glass will produce
many thousand neutrons per year. Neutrons from this interaction will enter the argon and could produce collisions identical to WIMP collisions. Neutrons which scatter multiple times or capture can be rejected because WIMPs will not scatter more than once. Otherwise the spatial reconstruction can reject some of the neutrons because neutrons from the PMTs are expected to interact near the edge of the detector while WIMPs can interact throughout.

In order to determine how effective the background cuts will be and determine the expected background after the cuts, a Monte Carlo simulation will be used to determine the final affects of the background neutrons. However, this Monte Carlo can only be effective if the neutron physics is simulated correctly throughout. In the rest of this Thesis, the interactions between neutrons and Argon implemented in MiniCLEAN's simulation software will be examined. Chapter 2 covers the background for the neutron physics examined, Chapter 3 describes the simulations used, Chapter 4 covers the analysis of elastic collisions between neutrons and Argon nuclei, Chapter 5 covers the inelastic collisions, and Chapter 6 covers neutron capture.
Chapter 2

Neutron Physics

In order to completely characterize the neutron backgrounds MiniCLEAN we must simulate neutrons interacting with all parts of the experimental apparatus. The simulations need to accurately depict how the neutrons will interact, meaning the simulated physics of all types of interactions must be checked to determine if there are any errors in the simulation. This chapter will summarize different aspects of neutron physics, including the expected results. Chapter 3 will introduce the simulation software and the simulations used to test the neutron physics.

2.1 Cross Sections

The most basic description of how particles interact is found in the cross section. The cross section between two particles describes how often the particles will interact, has units of area, and is inversely proportional to the path length. There are different cross sections for different interactions, for example the cross section for a neutron elastically scattering off a nucleus is different than for the neutron inelastically scattering. Cross sections are additive such that the two previously described cross sections can be added to give the cross section of the neutron elastically or inelastically scattering. In addition, cross sections vary strongly for different materials and are dependent on the energies of the interacting particles.

In this thesis I am interested in interactions between neutrons and the liquid
argon in the MiniCLEAN experiment. To find the cross sections between neutrons and argon nuclei we must examine neutrons passing through argon. Cross sections can be interpreted as a probability that a neutron will interact with the argon nuclei meaning, for a beam of neutrons, the number which will have not interacted can be described by the equation

$$\frac{dI}{dx} = -N\sigma I. \quad (2.1)$$

Here, $\sigma$ is the cross section, $I$ is the intensity of neutrons that have not scattered, $x$ is the distance traveled through the argon, and $N$ is the number density of the argon nuclei equal to

$$N = 2.1104 \times 10^{-3} \text{ atoms/barns mm}. \quad (2.2)$$

The barn is a unit of area equal to $10^{-24}$ cm$^2$ and is commonly used for cross sections. These specific units are used for ease with the simulation units. From equation 2.1 we can find how the intensity of unscattered neutrons is expected to change with respect to the distance traveled through a material:

$$I(x) = I_0 e^{-N\sigma x}. \quad (2.3)$$

The cross sections can be found experimentally by varying the distance the neutrons must travel in the argon, determining the number of neutrons which have not scattered, and then fitting to equation 2.3.

Figure 2-1 shows how the neutron cross sections for argon-40 vary with energy. Neutron energies are categorized into three types, thermal, resonance, and fast. These types are explained by the different interaction types that predominate at the different energies. For thermal neutrons, $E < 1$ eV for argon-40, neutron capture is the dominate process. Neutron capture is responsible for the difference between ENDF/B-VII.1 total and elastic at low energies. In the resonance energy range of $1$ keV $< E < 4$ MeV, the dominate elastic cross sections exhibit numerous sharply peaked resonances. Figure 2-3 shows some of the neutron elastic cross section resonances. Fast neutrons
Figure 2-1: A log-log total neutron argon-40 cross section as measured by Winters et al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. The difference between the ENDF/B-VII.1 total and ENDF/B-VII.1 elastic at low energy is due to the neutron capture cross section. The significant difference between the ENDF/B-VII.1 inelastic and G4NDL4.0 inelastic is due to G4NDL4.0 including the (n,2n) and (n,3n) final states while ENDF/B-VII.1 does not. ENDF/B-VII.1 total includes elastic, inelastic, capture, (n,2n), and (n,3n).
Figure 2-2: A linear plot of the total neutron argon-40 cross section as measured by Winters et. al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. The significant difference between the ENDF/B-VII.1 inelastic and G4NDL4.0 inelastic is due to G4NDL4.0 including the (n,2n) and (n,3n) final states while ENDF/B-VII.1 does not. ENDF/B-VII.1 total includes elastic, inelastic, capture, (n,2n), and (n,3n).

are neutrons with energies above several MeV and have large inelastic cross sections, seen best in Figure 2-2. In Figures 2-1 and 2-2, the difference between ENDF/B-VII.1 Inelastic and G4NDL4.0 Inelastic is due to ENDF excluding some final states which are included by G4NDL, as explained in Section 2.3.

2.2 Cross Section Measurements

The most complete measurements of the neutron total cross section for argon-40 were taken by Winters et. al. at The Oak Ridge Electron Linear Accelerator in 1991[7]. A neutron beam was directed toward a steel cylinder filled with argon gas and the transmission rate of the neutrons was found. The total cross sections were measured for neutron energies between 0.007 MeV and 50 MeV. The data which were measured
Figure 2-3: A section of resonances of the total neutron argon-40 cross section as measured by Winters et. al. [7] compared to the ENDF/B-VII.1 and G4NDL4.0 databases. Argon-40 has a large resonance at about 50 keV which, while partially mitigated by the presence of argon-36, was not detected by the Winters et. al. experiment.

are plotted in Figures 2-1, 2-2, and 2-3. These three plots show three different views of the data. Also plotted are the data from two neutron cross section databases explained below.

Several features of the argon cross section are seen in Figure 2-3. Nuclear theory predicts a deep, wide resonance at around 50 keV due to interference between the different nuclear energy states. Figure 2-3 shows that this resonance is expected to have cross sections as low as $10^{-3}$ barns, but the Winters et. al. total cross section data are not nearly this low. This discrepancy is partially due to the presence of argon-36 in natural argon. Argon-36 has a large affect, even though natural argon is only 0.3% argon-36[16], because its cross section at 50 keV is nearly four orders of magnitude larger than argon-40.

The addition of argon-36 to create natural argon (neglecting the 0.06% that is argon-38) is plotted in green on Figure 2-3. This still does not account for the discrepancy between Winters et. al. data and the theoretical prediction. Other possible corrections between the predicted elastic cross section and the predicted
total cross section, the inelastic and capture cross sections, are zero or insignificant for all isotopes at these energies. The theories used to calculate the predictions have extensive experimental backing[6], meaning the difference between the prediction and the data does not invalidate the theory because the experimental difficulty in measuring cross section of that size is just as significant.

The deep resonance in the argon-neutron elastic cross section is interesting because it has the possibility of creating a monoenergetic neutron beam from a beam of low energy resolution because neutron which either start with that energy or scatter into that energy rarely interact while all other neutrons lose energy and capture.

2.3 Cross Section Databases

ENDF/B-VII and G4NDL are datasets which contain neutron cross sections for energy less than 20 MeV. ENDF/B-VII and G4NDL are created through the combination of available data, models, and theories.

The ENDF/B-VII is released by the National Nuclear Data Center and is maintained by the Cross Section Evaluation Working Group (CSEWG) and is considered the most accepted database for low energy neutron cross sections[6]. ENDF/B-VII was initially released in 2006 and an update, ENDF/B-VII.1, was released in Dec 2011. The database contains cross sections for 423 nuclides; the data for each nuclide includes some subset of cross sections for elastic, inelastic, capture, and fission interactions and their respective angular distributions. ENDF/B-VII.1 contains the total neutron cross section for argon-40 along with the elastic, inelastic, and capture cross sections. In addition to the total inelastic cross section, ENDF/B-VII contains the cross section and angular distribution for nine inelastic final states and for exciting argon to the first 25 energy levels. The different final states for the inelastic cross sections in ENDF/B-VII are plotted in Figure 2-4. This figure indicates, and it was numerically confirmed, that ENDF/B-VII does not include the (n,2n) or the (n,3n) states in its total inelastic cross section. This explains the difference between the ENDF/B-VII and G4NDL cross sections in figure 2-2. The combination of the
Figure 2-4: ENDF/B-VII.0 cross sections for the different final states of an inelastic collision between a neutron and an argon nucleus. Only the first six of the 25 \((n, n_k)\) states are shown in this plot. The plot also indicates that ENDF/B-VII does not include the \((n, 2n)\) and \((n, 3n)\) states in its total inelastic cross section.

ENDF/B-VII \((n, \text{inelastic})\), \((n, 2n)\), and \((n, 3)\) is compared to the G4NDL total inelastic neutron cross section in figure 5-1.

G4NDL is the neutron cross section dataset used by the GEANT4 simulation package[8] (see section 3.1). G4NDL is a combination of several different neutron databases including ENDF/B-VI, ENDF/B-VII, JENDL, ROSFOND, etc. Over the course of this work, there was a new version of G4NDL released through a new release in GEANT4. The older version, G4NDL3.13, was based primarily on ENDF/B-VI while the newer version G4NDL4.0 is primarily based on ENDF/B-VII. G4NDL does not include a complete total cross section but does have the elastic, inelastic, and capture cross sections. The G4NDL3.13 inelastic cross section contains seven final states while G4NDL4.0 contains eight. Both versions of G4NDL include the first 23 excited states of argon-40 and a continuum state to account for the rest. The inelastic final states for G4NDL4.0 are plotted in figure 2-5.
Figure 2-5: G4NDL4.0 cross sections for the different final states of an inelastic collision between a neutron and an argon nucleus. Only the first six of the 23 \((n, n_k)\) states are shown. G4NDL4.0 does not include data for the \((n, ^3\text{He})\) final state.
In addition to ENDF/B-VII and G4NDL, ENSDF (Evaluated Nuclear Structure Data File) contains nuclear excited state and decay information, including the released gamma rays, for thousands of nuclides[4]. Data from here were used in checking the energies of the gammas released during inelastic collisions and neutron capture.

2.4 Elastic Collisions and Angular Distributions

A two-body elastic collision is completely described by the center of mass scattering angle because, with this angle it possible to calculate the change in energy and momentum for every particle in the collision. The angular distribution for neutrons scattering off nuclei, or the probability of the neutron scattering at a given angle, depends on the initial energy of the neutron and the scattering target. The angular distribution can be calculated using several different physics models such as partial wave scattering or the Bohr approximation if the interaction potential between the particles is known[11]. For the purpose of this thesis the angular distributions were compared to those listed in the ENDF/B-VII and G4NDL databases.

To compare the angular distributions found in simulations to the distributions in the databases, the lab scattering angle must be converted into the center of mass scattering angle. The center of mass frame is used because the total momentum of the frame is always zero. In the center of mass frame,

\[ |p_{CM}| = |\vec{p}_{i,n}| = |\vec{p}_{i,Ar}| = |\vec{p}_{f,n}| = |\vec{p}_{f,Ar}|, \tag{2.4} \]

and the scattering angle is the same for both particles. This means understanding an elastic collision is only a matter of knowing the scattering angle.

Assuming the initial momentum of the neutron is entirely along the x-axis, which is possible in simulation, the center of mass scattering angle is

\[ \cos \theta_{CM} = \frac{p_{CM,x}}{|p_{CM}|} \tag{2.5} \]

where \( p_{CM,x} \) is the final momentum in the center of mass frame, found by
The angular distribution is experimentally determined by measuring the scattering angle of collisions with enough statistics to determine the probability of each possible angle.

The angular distribution of the simulated collisions will be compared to those listed in neutron physics databases. The probability densities from the ENDF/B-VII and G4NDL databases are listed as Legendre polynomial coefficients because Legendre polynomials are solutions to many central potential problems in spherical coordinates and partial wave scattering calculates angular distributions by expanding in Legendre polynomials. This makes Legendre a convenient choice for parameterizing angular distributions. The complete distributions were produced from the Legendre polynomial coefficients using the equation:

\[
P_l(\cos \theta_{CM}) = \sum_{i=0}^{NL} \frac{2l + 1}{2} a_i(E) P_l(\cos \theta_{CM})
\]

Where \( P_l \) is the Legendre polynomial of \( l^{th} \) order, \( a_0 = 1 \), and \( a_{l>0} \) are the coefficients listed in the ENDF/B-VII and G4NDL databases.

Once the angular distributions have been found, the expected distribution for quantities like the argon recoil energy can be calculated. The argon is initially stationary in the lab frame because we can disregard thermal motion which is on the order of meV. The argon recoil energy is the final kinetic energy of the argon:

\[
p_{LAB,x} = \gamma p_{CM,x} - E_{cm} \beta \gamma.
\]

The \( \gamma \) and \( \beta \) are for the Lorentz transformation between the Center of Mass frame and the Lab frame. The magnitude of the center of mass momentum is found using the Lorentz transformation invariant \( s \).

\[
s = (m_N + m_{Ar})^2 + 2m_{Ar}T_{N,i}
\]

\[
|p_{CM}| = \sqrt{\frac{(s - m_{Ar}^2)^2 - 4m_N^2m_{Ar}^2}{4s}}
\]
\[ T_{\text{recoil,Lab}} = E_{\text{Ar,Lab}} - M_{\text{Ar}}. \] (2.10)

Where \( E_{\text{Ar,Lab}} \) is the final energy of the argon in the lab frame, calculated though the Lorentz transform

\[ E_{\text{Ar,Lab}} = \gamma \sqrt{|p_{\text{CM}}|^2 + M^2_{\text{Ar}} + p_{\text{CM}} \cos \theta_{\text{CM}} \beta \gamma}. \] (2.11)

The argon recoil depends only on the center of mass scattering angle, initial kinetic energy of the neutron, and the mass of the two colliding particles. There is also a maximum possible recoil energy which, for an argon-neutron collision, is 9.63% of the kinetic energy of the neutron.
Chapter 3

Simulations

3.1 Simulation Software

All the simulations in this work were run using the Reactor Analysis Tool (RAT) software package[5]. This software combines the simulation software of GEANT4[8] and GLG4Sim[13] and the I/O capabilities of ROOT[22]. GEANT4 is designed to simulate particles passing through matter and is responsible for most of the physics information in RAT. The physics in GEANT4 is known to have errors for some hadronic processes and the simulations in this Thesis were run to detect and characterize these errors. The simulations were originally run using a RAT build with GEANT4.9.3.p01 but were rerun when GEANT4.9.5 was released in December 2011. A significant difference between the two versions of GEANT4 is that GEANT4.9.3.p01 implements G4NDL3.13 while GEANT4.9.5 implements G4NDL4.0. GEANT4 uses G4NDL to calculate low energy neutron physics so it is expected that all the neutron physics will match with the correct version of data in G4NDL. All simulations and analysis methods between the two versions of GEANT4 are identical.

The RAT simulation creates Root data files containing the tracks of each individual particle and gamma ray. Tracks were divided into steps where each step is terminated in a physical process, such as elastic scattering. The position, momentum, and kinetic energy of the particle as well as the physical process terminating the step are known for each step in the neutron track.
3.2 Argon Sheet Simulations

The hadronic physics in GEANT4 was tested using argon-40 as the target nucleus because the MiniCLEAN experiment will use Liquid argon as the target material for WIMP detection. The main set of simulations were of monoenergetic neutrons passing through a sheet of natural argon. Natural argon is 99.6% argon-40, meaning analysis had to take small amounts of argon-36 and argon-38 into account[16]. However, as the amounts of these isotopes are very small, the presence of Ar-36 and Ar-38 does not significantly affect the results.

The argon sheet simulations were able to focus on different hadronic physics because RAT and GEANT4 have the ability to turn different physics lists on and off. For each simulation, all hadronic physics except the one of interest were turned off.

3.2.1 Elastic Collisions

Elastic Collisions are those in which kinetic energy is conserved, meaning the particles are left unchanged throughout. Elastic collisions between a neutron and an argon nucleus are of interest because these collisions resemble the collision expected between a WIMP particle and an argon nucleus. Since detection of WIMPs occurs through the scintillation caused by recoiling argon nuclei, it will be necessary to find how often argon nuclei are expected to recoil due to collisions with neutrons. The physics of the elastic processes implemented in the different versions of GEANT4 was examined to ensure these collisions were implemented properly.

To study the elastic hadronic processes a sheet of argon was simulated with monoenergetic neutrons passing through the sheet. Three different neutron energy ranges were simulated: 40 keV to 60 keV in 0.5 keV increments, 80 keV to 110 keV in 0.5 keV increments and 0.2 MeV to 25 MeV in 0.2 MeV increments. For each energy, 100,000 neutrons were simulated to obtain sufficient statistics for analysis. The neutron tracks were used to determine the cross section and angular distribution of an elastic collision between a neutron and an argon-40 nucleus. The conservation of momentum and conservation of energy was also checked for each collision. Analysis
of the elastic simulations is found in Chapter 4.

3.2.2 Inelastic Collisions

Inelastic collisions are collisions where kinetic energy is not conserved, meaning energy is transferred into other forms. In inelastic collisions between a neutron and an argon nucleus additional or different particles and gamma rays are often produced. For example:

\[ {^{40}\text{Ar}}_\text{18} + {^1_0}\text{n} \rightarrow {^1_1}\text{p} + {^{40}\text{Cl}}_\text{17} \]

is a possible result of an inelastic collision between an argon nucleus and a neutron. Gamma rays are often released during an inelastic collision and in the subsequent decays to ground states of the collision products.

The sheet of argon was also used to study simulated inelastic collisions. Monoenergetic neutrons of energies between 0.2 MeV and 20 MeV in intervals of 0.2 MeV were tracked passing though the argon sheet. Lower energy simulations were unnecessary because the inelastic cross section is zero for energies less than 1.49 MeV. One million neutrons were simulated for each energy because higher statistics were needed to see effects of some final state cross sections, which were significantly more rare than elastic scattering. The neutron tracks were used to find the cross section, angular distribution, and final state of each inelastic collision. The gamma rays released and decay scheme of excited argon-40 were checked as well as the conservation of energy and momentum. Analysis of the inelastic collisions is found in Chapter 5.

3.2.3 Neutron Capture

Neutron capture occurs when a neutron collides with a nucleus and is absorbed in the nucleus. If a neutron does not escape from a detector, it is most likely to be captured because, as a neutron scatters in a material it loses energy and lower energy neutrons (E \textless; 1 eV) have the highest neutron capture cross section. This process always releases the same amount of energy, since the conversion between a neutron
and argon-40 to argon-41 always lowers the total nuclear binding energy by the same amount. While the individual gammas released during a neutron capture are not always identical, the accumulated spectrum over many captures is specific to the target nucleus[4]. A neutron captured in argon-40 creates argon 41 which is unstable and will later decay with a half life of 109.61 minutes[4].

Neutron Captures were studied with a sheet of argon using monoenergetic neutrons of energies between 1e-11 and 1e1 MeV with four evenly spaced energies per order of magnitude. In addition, energies surrounding two resonances were also studied. For each energy, 100,000 neutrons were simulated to obtain sufficient statistics. The particle track information was used to determine the capture cross section, the argon 41 half life and decay scheme, and the gammas released on capture. Analysis of the neutron captures is found in Chapter 6.
Chapter 4

Elastic Collisions

Elastic collisions, which conserve kinetic energy, were simulated using GEANT4.9.3.p01 and GEANT4.9.5. Three energy ranges were examined: 40-60 keV, 80-110 keV, and 0.2-25 MeV. Using neutron tracts from these simulations, the effective elastic cross sections and the angular distributions of the collisions were found. In addition, the conservation of energy and momentum was examined to catalog any non-physicalities occurring in the simulations.

4.1 Elastic Cross Section

The distance each simulated neutron traveled through the argon sheet before colliding elastically was found to determine the effective elastic cross sections in the RAT simulations. The fraction of neutrons which had not interacted with the argon was calculated as a function of distance within the sheet. This fraction was fit to the expected exponential decay function (see section 2.1), where the elastic cross section was a fit parameter. The effective cross sections are shown in Figures 4-1, 4-2, and 4-3. The simulated elastic cross sections agree with their corresponding GEANT4 and G4NDL versions, including energies which lie on resonances in the two lower energy sets. However, G4NDL4.0 matches the data from ENDF/B-VII much more closely than G4NDL3.13. ENDF/B-VII and G4NDL4.0 both contain elastic resonance information up to 5 MeV while G4NDL3.13 only contains resonances up to
Figure 4-1: The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 0.2 and 22 MeV in 0.2 MeV intervals. The simulations implementing GEANT4.9.3 match the G4NDL3.13 data and the simulations implementing GEANT4.9.5 match the G4NDL4.0 data. G4NDL3.13 only includes resonances up to 1 MeV while G4NDL4.0 and ENDF/B-VII includes resonances up to 5 MeV.

about 1 MeV. In addition, G4NDL3.13 does not include all the resonances which are in ENDF/B-VII that are less than 1 MeV.

The effective cross sections for both sets of simulations are discontinuous at 20 MeV (Figure 4-1). This discontinuity is due to a change in the simulated physics governing the collisions at that point. Below 20 MeV, elastic scattering is determined via the differential cross section data using the GEANT4 neutronHP method. Above 20 MeV the Glauber model is used to calculate the cross section and angular distribution[10]. For argon-40 this produces a discontinuous cross section at 20 MeV, although other elements may not experience such a discontinuity.

### 4.2 Angular Distribution

The angular distributions of the elastic collisions were found by tracking the trajectory changes of each neutron before and after an elastic collision as described in section 2.4. The angular distribution of an elastic collision between an 8 MeV neutron and an argon-40 nucleus is plotted for GEANT4.9.3.p01 and GEANT4.9.5 in figure 4-4. The simulation data was normalized to one event total. The data from ENDF/B-
Figure 4-2: The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 40 and 60 keV in 0.5 keV intervals.

Figure 4-3: The simulated neutron-argon elastic scattering cross section for neutrons with initial energies between 80 and 110 keV in 0.5 keV intervals.
Figure 4-4: The angular distribution of the outgoing neutron during an elastic collision between an argon nucleus and a neutron with 8 MeV of energy. The plots are normalized to one event. The ENDF/B-VII and G4NDL distributions were built from their Legendre coefficients. The simulations match the respective versions of G4NDL and G4NDL4.0 is more similar to ENDF/B-VII.

VII, G4NDL3.13, and G4NDL4.0 are all created from Legendre coefficients as also described in section 2.4. As with the elastic cross sections, the RAT simulations match their respective versions of GEANT4 and G4NDL, but G4NDL4.0 matches ENDF/B-VII.

The argon recoil energy was found in the simulation as well as calculated from the scattering angle of each collision. The two values are compared in Figure 4-5 for GEANT4.9.3.p01 and GEANT4.9.5. The argon recoil energy is consistent with the scattering angle in each simulation.

### 4.3 Energy and Momentum Conservation

The total change in energy and momentum of each collision was determined to find any strange behavior present in the simulations. For this section the change in energy and the change in momentum are defined as:

\[
\Delta E = E_{Ar, final} + E_{n, final} - E_{n, initial}
\]

\[
\Delta \vec{p} = \vec{p}_{Ar, final} + \vec{p}_{n, final} - \vec{p}_{n, initial}
\]

where the energies are all kinetic energies in the lab frame. The initial energy of the
Figure 4-5: The nuclear recoil energy deposited by the initial 5.0 MeV neutron during the elastic collision. The blue markers indicate the energy information in the simulation and the black markers indicate the recoil energy calculated from the simulated scattering angle. The initial neutrons had 5 MeV of kinetic energy. The plots are normalized to one event.

argon-40, due to thermal motion at 87K is expected to be on the order of meV and is therefore insignificant. Any relativistic corrections are unnecessary because the largest Lorentz \( \gamma \) in these simulations is 1.000013.

The change in energies for the simulations with initial neutron energy of 8 MeV are plotted in Figure 4-6. From Figures 4-6(c) and (d), the change in energy is proportional to the scattering angle. This is extremely odd because there is no obvious reason for the change in energy to resemble the angular distributions. Every elastic collision results in approximately 100 eV too much kinetic energy. This discrepancy is smaller in GEANT4.9.3.p01 where the GEANT4.9.3.p01 change in energy is about one fifth the change in energy in GEANT4.9.5.

In addition to the change in energy, the change in momentum of elastic collisions was also studied. The magnitude of the change in momentum for the 8 MeV neutron simulations is plotted in Figure 4-7 (a) and (b). The magnitude in the change is momentum is about 0.01% of the initial momentum, however it is interesting that the peak in momentum non-conservation which is around 0.04 MeV/c is in the same location for elastic and inelastic collisions (see section 5.4). Figure 4-7(c) and (d) indicate the direction of the change in momentum vector, momentum non-conservation is nearly isotropic but slightly biased along the xy-axis.
Figure 4-6: (a) and (b) are the change in energy for 8.0 MeV neutron simulations in GEANT4.9.3.p01 and GEANT4.9.5. (c) and (d) are the change in energy versus the cosine of the scattering angle which is a linear relationship for some unknown reason. The plots are normalized to one event. The width of the distribution increases in GEANT4.9.5 but the shape remains the same.
Figure 4-7: (a) and (b) are the magnitude of the change in momentum vector for the 8.0 MeV neutron simulations in GEANT4.9.3.p01 and GEANT4.9.5. (c) and (d) represent the direction of the change in momentum vector which is nearly isotropic. The plots are normalized to one event.
Figure 4-8: The change in momentum versus the change in energy for the 8 MeV simulations from GEANT4.9.3.p01 and GEANT4.9.5. The plots are normalized to one event.

Figure 4-8 shows the change in momentum compared to the change in energy. The plot shows two distinct populations of events separated by the change in energy of the collision.

4.4 Summary

The effective cross section and angular distribution of the simulated elastic collisions are in good agreement with the G4NDL data on which the simulations are based. The energy and momentum of the collisions are not conserved, although the magnitude of the energy non-conservation is smaller for GEANT4.9.3.p01 than for GEANT4.9.5. The change in energy of the collisions is proportion to the angular distribution despite no physical reason for this to be the case. The change in momentum direction is nearly isotropic and has a bimodal relationship to the change in energy.
Chapter 5

Inelastic Collisions

Monoenergetic neutrons were simulated traveling through a sheet of natural argon in order to verify the simulated physics of a neutron inelastically scattering off an argon-40 nucleus. Hadronic elastic physics and neutron capture physics were turned off, leaving only inelastic collisions between an argon nuclei and a neutron. One set of energies from 0.2 MeV to 20 MeV in intervals of 0.2 MeV was simulated with $10^6$ neutrons per energy. The neutron tracks were used to find the inelastic cross section and the angular distributions of the collisions. The products of the collisions were used to classify the final state, allowing for the analysis of the final state cross sections and argon-40 excitations and decay schemes. The conservation of energy and angular momentum was again determined in order to examine any simulation discrepancies.

5.1 Total Inelastic Cross Section

The distance each simulated neutron traveled through the argon sheet was determined and used to calculate the effective inelastic cross sections in GEANT4. The fraction of neutrons which had not interacted with the argon was found as a function of the distance traveled. This fraction was fit to the expected exponential decay function (see section 2.1), where the total inelastic cross section was a fit parameter.

The total inelastic cross section was found for each simulated neutron energy and is plotted in Figure 5-1. The (n,2n) and (n,3n) final states of ENDF/B-VII.1
Figure 5-1: The total inelastic cross section of argon-40 found in the RAT simulations compared to the well accepted values from ENDF/B-VII.1 and G4NDL3.13 or G4NDL4.0. The (n,2n) and (n,3n) states of ENDF/B-VII.1 are added to the (n,inelastic) values because ENDF/B-VII.1 does not include these states in the total cross section.

...are added to the (n,inelastic) state for comparison because ENDF/B-VII.1 does not include these states in the total inelastic cross section while GEANT4 and G4NDL4.0 do include these states.

The effective total inelastic cross sections lie along G4NDL3.13 for GEANT4.9.3.p01 and along G4NDL4.0 for GEANT4.9.5. This is expected because GEANT4 uses G4NDL while implementing low energy neutron physics in the NeutronHP physics model. The G4NDL3.13 cross sections are approximately 70% the size of ENDF/B-VII while G4NDL4.0 cross sections are similar to the ENDF/B-VII.

5.2 Inelastic Final States

An inelastic collision between a neutron and an argon-40 nucleus can result in several different final states, listed in Table 5.1. Each type of collision is denoted as \((X,Y)\) where \(X\) is the incident particle and \(Y\) is/are the final product(s). The target, argon-40, and the larger products, such as sulfur-37 or chlorine-40, are implicit. The \((n,n_k)\) states indicate a collision where the argon nucleus has been excited to the energy state \(k\). The individual \((n, n_k)\) states, distinguished using the released gamma rays,
Table 5.1: The unique decay products created during inelastic scatters. These were used to determine what type of inelastic scatter had occurred.

are described in Section 5.3.

The unique products, listed in Table 5.1, were used to classify each collision, however those chosen products cause some error due to the presence of argon-38 in the simulation. However, since argon-38 accounts for only 0.06\% of natural argon and those collisions resulted in different final states, these effects were easily negated.

Table 5.1 also shows the labels used for the final states by G4NDL4.0. G4NDL3.13 does not include the (n,t) and (n,^3He) final states for argon-40 while G4NDL does not include the (n,^3He) final state. This is likely due to the size of these cross sections, (n,t) is less than $10^{-3}$ barns and (n,^3He) is less than $10^{-6}$ barns for all neutron energies less than 20 MeV.

5.2.1 Cross Sections of Final States

The cross sections for each final state were found by determining the fraction of inelastic collisions which resulted in the unique decay product for the final state. The effects due to argon-38 could be removed by determining all products of the collision instead of just one product. The cross section of the final state is then

$$\sigma_{FS} = \sigma_{inelastic} \times \frac{\text{Number in Final State}}{\text{Number of Inelastic Collisions}} \quad (5.1)$$

Figure 5-2 shows the cross sections for the (n,2n) and (n,\alpha) final states for GEANT4.9.3.p01.
Figure 5-2: The cross section of the final states \((n,2n)\) and \((n,\alpha)\) for GEANT4.9.3.p01 and GEANT4.9.5. The simulations lie along G\(4\)ND\(L\)3.13 or G\(4\)ND\(L\)4.0 while G\(4\)ND\(L\)4.0 matches ENDF/B-VII.1.
5.2.2 Angular Distribution

In addition to the cross sections, the angular distributions of each final state were also examined. The angular distributions for simulations using GEANT4.9.3.p01 are completely isotropic, the scattering angle for each particle is independent of all other particles. This is consistent for G4NDL3.13, which includes no data regarding the angular distributions of any final state and thus sets these distributions to be isotropic.

G4NDL4.0 and ENDF/B-VII include energy dependent non-isotropic distributions for the \((n,n_k)\) final states and analysis of the GEANT4.9.5 simulations show non-isotropic distributions for these states. Figure 5-3(a) shows the angular distribution of the \((n,n_1)\) state for 7 MeV initial neutrons compared to the expected distributions from G4NDL4.0 and ENDF/B-VII. Oddly, the simulated angular distribution matches ENDF/B-VII better than G4NDL4.0 with a \(\chi^2\) of 2.22 compared to

Figure 5-3: The angular distribution of the neutron in the inelastic collision in the GEANT4.9.5. The angular distribution is isotropic for all final states except the \((n,n_k)\) states. (a) is the \((n,n_1)\) final state for 7.0 MeV neutrons which is non-isotropic and has a distribution that depends on the initial energy of the neutron and (b) is the \((n,2n)\) final state which is expected to be isotropic. The plots are normalized to one event.

and GEANT4.9.5. The cross sections for each of the final states lie along the G4NDL3.13 or G4NDL4.0 data as expected. G4NDL4.0 is identical to the widely accepted ENDF/B-VII.1 values for the individual final state cross sections while G4NDL3.13 is generally different from ENDF/B-VII.
Figure 5-4: The total energy of the gamma rays released during an inelastic collision with an initial neutron energy of 3.8 MeV or 7.0 MeV. The total gamma energy represents the final energy state of the argon-40 nucleus. The GEANT4.9.3.p01 states are extremely non-physical. The expected energy levels are listed in Table 5.2.

to 7.38.

All final states other than \((n, n_k)\) simulated in GEANT4.9.5 have isotropic distributions and G4NDL4.0 does not list any angular distributions for these final states. ENDF/B-VII explicitly lists \((n,2n)\), \((n,3n)\), \((n,n\alpha)\), and \((n,np)\) as isotropic and includes no data for the other final states. Figure 5-3(b) is the angular distribution for the \((n,2n)\) final state for initial neutrons with 12 MeV of kinetic energy. This distribution is completely isotropic, meaning the scattering angles of the two final neutrons are completely independent.
5.3 Excited States and Gamma Rays

The gamma rays released during the inelastic collision and any subsequent decays of the argon-40 nucleus were examined to check the cross sections for the \((n,n_k)\) final states and the decay scheme of the immediate argon-40 deexcitation.

The final energy state of the argon-40 nucleus was found by determining the total energy of all gammas released by the nucleus. Figure 5-4 shows the total gamma energy released in a collision where the final state is \((n,n_k)\) in GEANT4.9.3.p01 and GEANT4.9.5 for initial neutrons with energy 3.8 MeV and 7.0 MeV. The \((n,n_k)\) final states show a significant difference between GEANT4.9.3.p01 and GEANT4.9.5. Since the total gamma energy released represents the energy state to which the argon-40 nucleus was excited, the total gamma energy should be discrete states such as in Figure 5-4(b) from GEANT4.9.5. The total gamma energy released in GEANT4.9.3.p01, Figure 5-4(a), has an extremely nonphysical square distribution about 1 MeV wide that ends at the expected energy of each excited state. Figure 5-4(c) shows the effect of these square distributions at higher energies when the widened states stated overlapping. The switch from GEANT4.9.3.p01 to GEANT4.9.5 was completely necessary to fix the total released gamma energy.

Figure 5-4(d) shows an effect of implementing excitation states in a simulation. G4NDL4.0 and ENDF/B-VII includes the first 25 discrete energy states which are below 4.69 MeV and then has a continuum state above 4.69 MeV. This is because the higher energy states are very close together such that it is difficult and unnecessary to determine the exact state. The cross sections for individual energy states were found by counting the fraction of collisions which resulted in the correct amount of gamma energy released. The cross sections for the first five energy states are shown in Figure 5-5 and are in good agreement with the G4NDL4.0 values. These cross sections were not found using the GEANT4.9.3.p01 simulations because the wide non-physical distributions for each energy level made the implemented analysis method impossible at higher energies.

In addition to the total gamma energy released, the individual gamma rays were
examined to determine if the gamma rays had the correct energy values and existed in the correct proportions. The analysis of the decay scheme and branching ratios was only completed for the GEANT4.9.5 simulations due to the non-physicalities in the GEANT4.9.3.p01 simulations. Table 5.2 shows the energy levels and gammas for the first five excited states of argon-40 given in ENDSF and G4NDL4.0. The data from G4NDL4.0 is the same as the data in G4NDL3.13. G4NDL4.0 has a 2129keV gamma and a 2892keV gamma which do not exist in ENDSF, but these two lines are only created about 1% of the time and are not extremely significant. In addition, G4NDL4.0 has a 682keV gamma which represents a transition from the fifth state to the third state while the corresponding 1087keV gamma in ENDSF is a transition from the fifth state to the second state. For the excited states above the first excited state, the most common transition is the transition to the first excited state which then decays to the ground state. Due to this fact, it is expected that there will be large quantities of 1460 keV gamma rays produced during \((n,n_\gamma)\) collisions.

For this analysis, the first five excited states of the argon-40 nucleus were examined and any gamma rays which came from collisions with argon-38 or argon-36 were ignored. The number of each gamma ray released was found and the decay lines where
<table>
<thead>
<tr>
<th>Excited State</th>
<th>Energy Level (ENSDF)</th>
<th>Energy Level (G4NDL4.0)</th>
<th>Gammas (ENSDF)</th>
<th>Ratio</th>
<th>Gammas (G4NDL4.0)</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1460.9</td>
<td>1460.9</td>
<td>1460.8</td>
<td>100</td>
<td>1460.8</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>2120.8</td>
<td>2120.8</td>
<td>650.1</td>
<td>100</td>
<td>659.9</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2129.7</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>2524.1</td>
<td>2521.1</td>
<td>1063.1</td>
<td>100</td>
<td>1063.2</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2524.1</td>
<td>75</td>
<td>2524.0</td>
<td>75.4</td>
</tr>
<tr>
<td>4</td>
<td>2892.6</td>
<td>2892.6</td>
<td>369.0</td>
<td>1.0</td>
<td>368.5</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1431.8</td>
<td>100</td>
<td>1431.7</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2892.5</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>3208.0</td>
<td>3208.0</td>
<td>315.0</td>
<td>1.0</td>
<td>315.4</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1087.6</td>
<td>2</td>
<td>682.9</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1746.5</td>
<td>100</td>
<td>1747.1</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3208.2</td>
<td>11</td>
<td>3207.9</td>
<td>11.1</td>
</tr>
</tbody>
</table>

Table 5.2: The energy levels of argon-40 as listed in ENSDF and G4NDL4.0, as well as the gammas released during de-excitation and their branching ratios. All energies in keV. The different gamma energies in the fifth excited state, 1087.6keV and 682.9keV, are different transitions to the second and third state respectively.
Table 5.3: The ratios of all gammas created in the GEANT4.9.5 simulations with energies less than 3.6 MeV. All energies in keV and all errors are from statistics of simulation compared against the expected values. Table 5.3 contains the ratios in which the gammas where created compared to the ratios given in G4NDL4.0. The ratios were calculated from all gammas released in all simulations with an initial neutron energy less than 3.6MeV and the errors on the ratios are from the statistics of the simulation. There are several gammas which are made slightly more often than dictated by the G4NDL4.0 data however the deviation is small enough that it should not cause any significant issues in a full experiment simulation.

The entire decay scheme for the first five states for all simulations with energy less than 3.6MeV was also examined. The expected gammas were all created in correct numbers, for example for every $5^-\rightarrow 3^-$ transition there was a corresponding $3^-\rightarrow 1$ or $3^-\rightarrow 0$ transition.

Figures 5-6(a) and 5-6(b) are plots of all gammas released during an inelastic collision of a 4.0 MeV neutron with argon-40 for the GEANT4.9.3.p01 and GEANT4.9.5 simulations respectively. Figures 5-6(c) and 5-6(d) are the same plots on a log scale. The GEANT4.9.3.p01 simulation shows some flat distributions where there should be discrete lines but the GEANT4.9.5 simulation has all the expected gamma in the correct proportions at the correct energies.
Figure 5-6: Gamma rays released during the deexcitation of argon-40 excited by an inelastic collision with a 4.0 MeV neutron. (a) and (b) show the entire spectrum while (c) and (d) are semi-log plots of (a) and (b). The expected energies of the expected gamma rays are listed in Table 5.2. (e) and (f) are zoomed to show gammas with energy less than 5 keV. All plots are normalized to one event.
Figures 5-6(e) and 5-6(f) are plots zoomed to only show the gammas between 0 and 5 keV and show the only major anomalous behavior present in both GEANT4.9.3.p01 and GEANT4.9.5. Both versions have significant numbers of gammas released which have a non-physical energy below 5 keV. In the GEANT4.9.3.p01 simulation nearly 100% of the collisions had one extra small gamma ray. In the GEANT4.9.5 4.0 MeV neutron simulation, 30% of all created gammas were below 5 keV and there is an average of one non-physical gamma ray per two collisions. In both GEANT4.9.3.p01 and GEANT4.9.5 these small gamma rays are always created before the gammas with the correct energies.

The distribution of these low energy gammas is always cut off at 1 keV for the GEANT4.9.5 simulation and has a width proportional to the energy of the initial neutrons for neutrons less than 5 MeV. Above 5 MeV the width of the distributions does not vary with initial neutron energy. Since the 1 keV cutoff is different between GEANT4.9.3.p01 and GEANT4.9.5 it is possible this is a new restriction in GEANT4.9.5. This could also partially explain the discrepancies in energy conservation discussed in Section 5.4.

5.4 Energy and Momentum Conservation

Energy and momentum conservation were examined using the same definitions of change in energy and change in momentum used for the elastic collisions (equation 4.1). These definitions do not account for any changes in mass due to final states with particles which are different than the initial neutron and argon nucleus. For these final states, the change in energy due was found to be approximately the change in mass. The (n,n\textsubscript{k}) states were examined in more depth to determine if energy and momentum in these collisions were correctly conserved.

Figure 5-7 shows the total change in energy for 3.0 MeV and 5.0 MeV neutrons for GEANT4.9.3.p01 and GEANT4.9.5. The GEANT4.9.3.p01 simulations are evenly distributed around $\Delta E = 0$ for energies less than 4.69 MeV but become highly unrealistic once the continuum final state begins. The distributions get wider with increasing
Figure 5-7: The change in energy for the (n,\n\textsubscript{n}) states from the 3.0 MeV and 5.0 MeV simulations using GEANT4.9.3.p01 and GEANT4.9.5. All plots are normalized to one event.
energy and the tails on the distribution for the 5.0 MeV simulation (Figure 5-7(c)) are due to the continuum final state. The 3.0 MeV and 5.0 MeV GEANT4.9.3.pOl simulations had inelastic collisions with zero change in energy less than 0.2% of the time, meaning conservation of energy was rarely correct.

The GEANT4.9.5 simulations have a non-uniform distribution which could be due to the cutoff energy in the small gammas in Figure 5-6. The change in energy has sharp jumps at every integer keV, which correlates with the small gammas only occurring if they are greater than 1 keV. For neutrons below 4.69 MeV, the change in energy in the GEANT4.9.5 collisions is always negative, energy only disappears. After the continuum state begins at 4.69 MeV, positive energy changes begin to appear. In addition, the 3.0 MeV GEANT4.9.5 simulation had a net zero change in energy for 10% of the collisions and the 5.0 MeV GEANT4.9.5 simulation had a net zero change in energy for 25% of the collisions. This is much higher than GEANT4.9.3.pOl indicating that energy is likely better conserved in GEANT4.9.5.

Figure 5-8 shows the initial energy of the neutron subtracted from the final energy. For a (n,nk) collision where the neutron contains all the initial energy and no energy is gained from broken nuclear bonds, this quantity can not be positive if energy is going to be conserved. Figure 5-8(a) indicates that GEANT4.9.3.pOl breaks energy conservation by as much as 10 MeV in collisions where the initial neutron energy
is 10 MeV. The distinct lines in Figure 5-8(a) are also non-physical because there is a quasi-elastic component to every inelastic collision which imparts some recoil energy to the argon. The quasi-elastic aspect of each collision would smooth out the discrete lines from the inelastic component of the collision in the total distribution. The update from GEANT4.9.3.p01 to GEANT4.9.5 corrected the extreme breaks in energy conservation as shown in Figure 5-8(b) which has a physically possible distribution for the change in neutron energy.

The magnitude of the change in momentum is plotted in Figure 5-9 for neutrons with initial energy of 9.0 MeV from GEANT4.9.3.p01 and GEANT4.9.5. Both simulations show a peaked distribution centered around 0.04 MeV/c however, the GEANT4.9.5 simulation has a large spike at 0.04 MeV/c that is over twice the height of the rest of the distribution. In addition, the direction of the change in momentum vector is isotropic for both GEANT4.9.3.p01 and GEANT4.9.5 simulations.

Due to the possible connections between energy non-conservation and the small non-physical gammas, I looked to see if there were any more correlations between the small gammas and conservation of momentum and energy. It was hypothesized that the non-physical gammas could be created by the simulation in an attempt to fix energy non-conservation. Figures 5-10 and 5-11 show these correlations for the 5.0 MeV simulations using GEANT4.9.3.p01 and GEANT4.9.5 respectively. In Figure 5-10 plots (a) and (c) the number of gammas less than 10 keV is plotted versus the
Figure 5-10: The correlations between number and energy of the small gammas, the change in energy, and the change in momentum for the \((n,n')\) final states only of the 5.0 MeV GEANT4.9.3.p01 neutron simulation. The number, (a), and energy, (b), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in energy for the collision. The number, (c), and energy, (d), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in momentum for the collision. (e) is the change in energy of the collision compared to the change in momentum of the collision.
change in energy and the change in momentum, since the number of small gammas is nearly always one, there is no correlation between the number of small gammas and the resulting non-conservation of energy and momentum. Figure 5-10(b) shows the energy of each gamma which is less than 10 keV compared to the change in energy. While there is a slight correlation between higher energy gammas and a lower change in energy, meaning the gammas could correct some of the energy non-conservation, the effect is small if there at all.

In Figure 5-10(d), the energy of each small gamma is compared to the change in momentum, here there is a linear correlation between the two variables. This correlation implies that the addition of these small gamma rays is responsible for the non-conservation of momentum. This linear correlation is also present in GEANT4.9.5 however Figure 5-11(d) also shows there is now a proportionally more events which occur outside this correlation. In addition, the gammas outside the linear correlation occur more often for the discrete (n,nk) states as opposed to the continuum states.

In comparison to the GEANT4.9.3.p01 simulations, conservation of energy seems to be much more strongly connected to the low energy gammas in the GEANT4.9.5 simulations. In Figures 5-11 (a) and (c) the number of small gammas is compared to the change in energy and change in momentum in the collision. Figure 5-11(a) shows that the higher the number of non-physical gammas, the better energy is conserved and Figure 5-11(c) demonstrates that a larger number of gammas leads to worse conservation of momentum. Thus it is possible that the non-physical gammas in GEANT4.9.5 are an attempt to correct for energy non-conservation.

A visual comparison between Figures 5-10(b) and 5-11(b) shows that the number of gammas above about 4 keV has significantly increased between GEANT4.9.3.p01 and GEANT4.9.5. The same occurs in Figures 5-10(d) and 5-11(d) for the gammas outside the linear correlation. It is possible that there are two sources of these low energy gammas rays and between GEANT4.9.3.p01 and GEANT4.9.5 the predominate source switched.
Figure 5-11: The correlations between number and energy of the small gammas, the change in energy, and the change in momentum for the (n,nk) final states only of the 5.0 MeV GEANT4.9.5 neutron simulation. The number, (a), and energy, (b), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in energy for the collision. The number, (c), and energy, (d), of gammas with energy less than 10 keV released during an inelastic collision compared to the change in momentum for the collision. (e) is the change in energy of the collision compared to the change in momentum of the collision.
5.5 Summary

The total inelastic cross section and final state cross sections are consistent with the correct G4NDL versions. The angular distributions of the non-isotropic final states oddly match ENDF/B-VII better than the G4NDL data. The total gamma energy released after a \((n,n_k)\) collision indicates GEANT4.9.3.p01 has energy states with non-physical widths while GEANT4.9.5 has a correct amount of total gamma energy released. For GEANT4.9.5 the entire argon-40 deexcitation scheme is consistent with G4NDL4.0.

The individual gammas released during the deexcitation of argon-40 includes several flat distributions for GEANT4.9.3.p01 but is correctly discrete in GEANT4.9.5. Both GEANT4.9.3.p01 and GEANT4.9.5 have a significant number of non-physical gammas which are less than 5 keV. The GEANT4.9.3.p01 distribution for these small gammas is peaked at 1 keV while GEANT4.9.5 has a sharp cutoff at that value.

Neither energy nor momentum is correctly conserved in GEANT4.9.3.p01 and GEANT4.9.5 however GEANT4.9.3.p01 often has grossly incorrect values for the final neutron energy while the conservation in GEANT4.9.5 is not as egregious. In addition, the non-physical small gammas improve energy conservation and worsen momentum conservation for GEANT4.9.5.
Chapter 6

Neutron Capture

Neutron capture was analyzed using simulated neutrons passing through an argon sheet with energies ranging from $10^{-11}\text{MeV}$ to $10\text{MeV}$ including several resonance energies. There were 100,000 neutrons simulated for each energy value. For these simulations elastic and inelastic collisions were turned off so that the only method of interaction between the neutrons and argon nuclei was capture. The neutron capture cross section, gammas released on capture, and the subsequent decay of argon-41 were examined to determine the simulation accuracy.

6.1 Cross Section

The capture cross section for neutrons interacting with argon-40 was found by tracing each neutron’s path through the argon sheet and determining the location of capture. From this the fraction of neutrons which had not captured versus distance was found and fit to the expected exponential decay function where the cross section was the fit parameter. The neutron cross section at each simulated energy is plotted in Figure 6-1 and is compared to G4NDL4.0 and ENDF/B-VII.1. As expected the simulation cross sections match well with G4NDL4.0. ENDF/B-VII.1 is extremely similar to G4NDL4.0, however, the height of the resonance cross section is always lower in ENDF/B-VII.1.

The simulated neutron capture cross sections for argon 40 are also plotted in
Figure 6-1: The simulated cross section for neutron capture compared to ENDF/B-VII.1 and G4NDL3.13 or G4NDL4.0. Errors on the data points are from simulation statistics.

Figure 6-2: The simulation cross section for neutron capture zoomed in on a sharp resonance and a softer resonance. The simulation cross section matches with the datasets from ENDF/B-VII.1 and G4NDL4.0. Errors on the data points are from simulation statistics.

Figure 6-2. These plots show the simulated cross sections at two resonances compared to G4NDL4.0 and ENDF/B-VII.1. The simulated cross sections generally agree with G4NDL4.0 and ENDF/B-VII.

6.2 Capture Gammas

When a neutron is captured by a nucleus, energy is released due to the change in mass of the system. For an argon-40 nucleus capturing a neutron, 6.209MeV of energy is expected to be released in the form of photons.
Figure 6-3: The individual gamma rays released on capture of a 1e-4 eV neutron compared to the expected spectrum from ENSDF. The spectrum from the simulation does not match the spectrum from ENSDF, the simulation has extra lines and is missing some from ENSDF.

\[ ^{40}\text{Ar} + ^{1}_{0}\text{n} \rightarrow ^{41}\text{Ar} + 6.209 \text{ MeV} \]  

(6.1)

In addition to the total gamma energy being slightly different from the expected value, the individual gamma rays released are significantly different than the expected. The spectrum of gammas released during capture is unique for every isotope capturing a neutron. Due to this uniqueness, thermal neutron capture is used to determine the isotope content of materials, meaning capture gamma ray spectra are generally well documented. The Evaluated Nuclear Structure Data File (ENSDF) contains information regarding the gamma rays released during thermal neutron capture for argon-40. The data are given as the intensity of the gamma lines relative to the most frequent gamma energy, meaning the number of gammas at a specific energy per 100 gammas released at the most frequent energy.

The data from ENSDF are plotted in Figure 6-3 with the correctly scaled gammas released during the 1e-10MeV neutron simulation. The simulation gamma rays are significantly different than the expected ENSDF data with some lines having a higher

71
intensity and others having a lower intensity. In addition, where these individual gammas come from in G4NDL4.0 could not be determined. There are no argon-40 files listed in the cross section final states folder and the GEANT4 physics manual does not explicitly list where the gammas are created[10]. There is no difference in gammas released between GEANT4.9.3.p01 and GEANT4.9.5.

6.3 Argon 41 Decay

The capture of a neutron by argon-40 results in an argon-41 nucleus which is unstable. The subsequent decay of argon-41, via beta decay, was also examined for the simulations. Argon-41 is unstable with a half-life of 109.61 minutes[16]. To determine the half life of argon-41 in the simulation, the time between the creation of an argon-41 nucleus and its decay was found for each neutron captured. The fraction of argon-41 nuclei still in existence versus time was determined and fit to the expected exponential decay. The fit parameter is the decay time which is related to the half life by a factor of ln 2. For all decays occurring in all simulation energies the half life of argon 41 was found to be $108.73 \pm 0.03$ minutes, 28 standard deviations away from the accepted value.

$$^{41}\text{Ar} \rightarrow ^{41}\text{K}^* + e^- + \bar{\nu}_e$$ (6.2)

In addition to half life, the decay scheme of the argon-41 nucleus was checked against the expected $\beta^-$ decay. Every argon-41 nucleus decayed into an excited Potassium nucleus and released an electron and an electron neutrino.

$$^{41}\text{K}^* \rightarrow ^{41}\text{K} + 1293 \text{ keV}$$ (6.3)

The excited Potassium nucleus then released a 1293 keV gamma ray to settle into its ground state. The decay scheme for the argon-41 nucleus matches exactly with the expected decay scheme[4].
6.4 Summary

The simulated neutron capture cross sections agree with G4NDL4.0 and ENDF/B-VII. While the total gamma energy released is correct the individual gamma rays are significantly different than the expected spectra for both GEANT4.9.3.p01 and GEANT4.9.5. The subsequent decay scheme for argon-41 is correct but the half-life of the isotope is many standard deviations away from the accepted value.
Chapter 7

Conclusions

The neutron physics implemented in GEANT4.9.3.p01 and GEANT4.9.5 was analyzed to characterize the accuracy of GEANT4’s simulation of elastic and inelastic collisions as well as neutron capture. Simulation accuracy is necessary for the Monte Carlo simulations of MiniCLEAN’s neutron background. While energy and momentum are not accurately conserved for any of the processes tested, energy conservation in GEANT4.9.3.p01 inelastic collisions is extremely incorrect.

The effective cross sections for elastic, inelastic, and capture physics are all consistent with the expected version of G4NDL, G4NDL3.13 for GEANT4.9.3.p01 and G4NDL4.0 for GEANT4.9.5. In addition the angular distributions for elastic and inelastic collisions resemble the G4NDL data however the inelastic distributions do not always exactly agree with G4NDL. Overall, G4NDL4.0 agrees with the widely accepted ENDF/B-VII data much better than G4NDL3.13.

Energy and momentum is not exactly conserved for any of the simulated processes, however some discrepancies are larger than others. In elastic collisions, the change in energy is proportional to the cosine of the scattering angle for both GEANT4.9.3.p01 and GEANT4.9.5. The size of the energy non-conservation in elastic collisions is approximately $10^{-4}$ the value of the initial energy of the neutron. Energy conservation for inelastic collisions in GEANT4.9.3.p01 is extremely incorrect with instances of total energy changes approaching 16 MeV when the initial neutrons are of only 5 MeV. Since these instances result in extra higher energy neutrons, they have the potential
to negatively affect the MiniCLEAN background simulations. Energy conservation is still incorrect for GEANT4.9.5 inelastic collisions, but only by a factor of $5 \times 10^{-3}$ times the initial energy of the neutron; this will be less significant in the MiniCLEAN background simulation.

In the inelastic collisions, the total gamma energy released during a $(n,n\gamma)$ collisions indicates GEANT4.9.3.p01 has energy states with non-physical widths while GEANT4.9.5 has a correct amount of total gamma energy released. For GEANT4.9.5 the entire argon-40 deexcitation scheme is consistent with G4NDL4.0. The individual gammas released during the deexcitation of argon-40 includes several flat distributions for GEANT4.9.3.p01 but is correctly discrete in GEANT4.9.5. Both GEANT4.9.3.p01 and GEANT4.9.5 have a significant number of non-physical gammas which are less than 5 keV. The GEANT4.9.3.p01 distribution for these small gammas is peaked at 1 keV while GEANT4.9.5 has a sharp cutoff at that value. In addition, the non-physical small gammas improve energy conservation and worsen momentum conservation for GEANT4.9.5.

During neutron captures, the total gamma energy released is correct but the individual gamma rays are significantly different than the expected spectra for both GEANT4.9.3.p01 and GEANT4.9.5. The subsequent decay scheme for argon-41 is correct but the half-life of the isotope is many standard deviations away from the accepted value.

While still not completely consistent with the laws of physics, GEANT4.9.5 has strongly improved the accuracy of the neutron collisions simulated in GEANT4.
Bibliography


