Modeling and simulation of neutron detectors for the transient reactor test facility

by

Wenkai Fu

B.S., Nanjing Univ. of Aero. and Astro., 2011
M.S., Nanjing Univ. of Aero. and Astro., 2014

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Department of Mechanical and Nuclear Engineering
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Abstract

The Transient REActor Test (TREAT) facility was restarted and will be used to test accident-tolerant fuels to improve nuclear reactor safety. In this work, alternative neutron detectors for use in core and with the hodoscope at the TREAT facility were modeled and simulated using different computational tools to understand the underlying physics.

The Hornyak button scintillation detector used in the original TREAT hodoscope to detect fast neutrons and its variants were evaluated using Geant4 to simulate the coupled nuclear and optical physics. The Hornyak-button model predicted an intrinsic efficiency of 0.35% for mono-directional fission neutrons and strong gamma-induced Cherenkov noise, which agree relatively well with the reported experimental observations.

The proposed variants use silicon photomultipliers to reduce Cherenkov noise and have optimized layered or homogenized scintillation volumes. The layered and homogenized variants with 5-cm length were predicted to achieve neutron-detection efficiencies of 3.3% and 1.3%, respectively, at a signal-to-noise ratio of 100.

Another candidate devices for the hodoscope are the actinide and hydrogenous microstructured semiconductor neutron detectors (MSNDs) evaluated using Geant4 and MCNP. With a sufficient rejection of the gamma noises, the $^{235}$U-filled and the hydrogenous MSNDs were predicted to yield neutron-detection efficiencies of 1.2% and 2.5%, respectively, at the length of 2 cm.

The micro-pocket fission detectors (MPFDs) were developed to detect in-core neutrons, and the electron collection process in such devices was evaluated using Garfield++-based computational routine. The high-performance Garfield++ application was developed using the built-in, optimized element-search techniques and a hybrid MPI and OpenMP parallelization scheme. The preliminary results indicated that the averaged deposited energy per fission fragment was 7.15 MeV, and the induced current occurred within 400 ns.
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Major Professor
Jeremy A. Roberts
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Chapter 1

Introduction and Background

1.1 Motivation

In December 2010, the United States Department of Energy (DOE) declared a need for a domestic transient testing capability to develop nuclear fuels [17]. Such a capability became more crucial after the Fukushima Daiichi nuclear accident in March 2011. After the accident, development of accident-tolerant fuels (ATFs) used in light water reactors (LWRs) was of high interest [18]. To reintroduce a domestic, transient-testing capability, two reasonable alternatives were reviewed and analyzed: to restart the Transient Reactor Test Facility (TREAT) reactor at Idaho National Laboratory (INL) and to modify the Annular Core Research Reactor (ACRR) at Sandia National Laboratories (SNL) [17]. After evaluation, it was decided to restart the TREAT facility in February 2014 [19].

Transient testing involves placing nuclear fuel or material into the core of a nuclear reactor and subjecting it to short bursts of intense, high-power radiation to simulate accident conditions [1]. Fuel meltdowns, metal-water reactions, thermal interaction between overheated fuel and coolant, and the transient behavior of ceramic fuel for high temperature systems can be investigated [20]. In particular, transient testing of nuclear fuels is needed to improve current nuclear-power plant performance and sustainability, to make next generation reactors more affordable, to develop nuclear fuels that are easier to recycle, and to
improve the proliferation resistance of fuel designs [1].

TREAT is one of the six nuclear transient reactor facilities worldwide, and the others are the Annular Core Research Reactor (ACRR, USA), the Nuclear Safety Research Reactor (NSRR, Japan), the CABRI (France), the Impulse Graphite Reactor (IGR, Kazakhstan), and the Bystry Impulsny Gravitovy Reaktor (Bigr, Russia) [13]. Among these facilities, TREAT may be the most versatile [1]. Its extraordinary capability for nuclear-heated transient testing comes from the brilliantly basic design and decades of incremental facility upgrades. TREAT’s wide transient power range, irradiation experiment vehicles (IEVs) that simulate specimen boundary conditions, in-situ instrumentation, and post-transient examination facilities produce a full-capability package able to address data needs for practically any reactor type or accident category [3]. Upon resumption of operations, TREAT can contribute to reactor safety by: 1) providing basic data to predict the safety margin of fuel designs and the severity of potential accidents, 2) serving as a proving ground for fuel concepts designed to reduce or prevent consequent hazards, and 3) providing nondestructive test data via neutron radiography of fuel samples irradiated in other test reactors [21].

1.2 Transient Reactor Test Facility

TREAT is an air-cooled, thermal, heterogenous research reactor designed to evaluate the performance of nuclear fuels and materials under conditions simulating overpower and undercooling situations [13]. It was designed by the Argonne National Laboratory and has been operated from February 1959 to April 1994 at INL, after which it was in a standby shutdown. During this operating period, TREAT was mainly used to test fast reactor fuels [13].

The key components of TREAT are shown in Fig. 1.1, which mainly consist of the core, the hodoscope, and the neutron radiography facility. The hodoscope and the neutron radiography facility connect to two slots opened by penetrating the shield wall and the graphite reflector, respectively. The hodoscope slot bridges the in-core channel created by the assemblies whose fuel region is replaced by the empty zircaloy frame [3]. The hodoscope is used to

\[1\text{Ref. [1] states there are four transient facilities, which exclude the ACRR and the Bigr.}\]
monitor the specimen’s behavior, e.g., melting or vaporization, during transient experiment. The hodoscope collimates and detects fission neutrons emitted by the fuel specimen. The response of the detectors provides time and spatial resolution of fuel motion during transients and in-place measurement of fuel distribution before and after an experiment. The neutron radiography facility is used during steady state operation and can examine specimens up to 15 feet in length [1]. During a neutron radiography experiment, optical and gamma camera systems can be used to record the reactive mechanisms [1].

Figure 1.1: Key components of TREAT, from Ref. [1].
1.2.1 Core

Shown in Fig. 1.2 is the top view of the TREAT core, reflector, and biological shielding. Summarized in Table 1.1 are the characteristics of the core design and components. The TREAT core consists of $19 \times 19$ (361) assemblies arranged in $4 \times 4$-inch$^2$ lattice with a height of 8 feet (about 2.4 m). The 361 assemblies are the control rods, the experiment assembly (IEV), the graphite reflector assemblies, and the fuel assemblies. The TREAT core can be configured by loading these assemblies into different positions for desired nuclear parameters or experimental objectives [3]. The configurable core, together with the versatile IEV design, represent TREAT’s flexible nature, which enables testing different fuel specimens in multiple accident scenarios. At the center of the core is a test hole through which the IEV is inserted. Typically, the IEV replaces one or two assemblies, thus, the irradiated volume is $4 \times 4$ inch$^2 \times 4$ feet (one assembly is replaced) or $4 \times 8$ inch$^2 \times 4$ feet (two assemblies are replaced). The core is reflected by about 2 ft. of graphite on all sides.

The fuel assemblies have 4-feet (1.2 m) active height in the middle. The fuel is 93.1% enriched high enriched uranium (HEU) of UO$_2$. The fuel is dispersed in a graphite matrix (about 1:10000 $^{235}$U/C atom ratio) [1], or 0.2 wt% $^{235}$U in the total fuel mixture [13]. The dilute distribution of uranium oxide in the fuel blocks rapidly transfers the transient heat into the graphite heat sink/moderator, which causes a neutron energy spectral shift with strong negative temperature feedback for safe self-limiting power excursions [3]. As part of the Materials Management and Minimization program, designing, qualifying, and fabrication of a new low enrichment uranium (LEU) core to substitute the original 60-year old HEU fuel core is under investigation [22].

Table 1.1: Core design and components of TREAT, after Ref. [13].

<table>
<thead>
<tr>
<th>Effective core height (cm)</th>
<th>122</th>
<th>Reactor driver fuel coolant</th>
<th>air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Driver fuel</td>
<td>UO$_2$</td>
<td>Enrichment (wt%)</td>
<td>93.1</td>
</tr>
<tr>
<td>Driver fuel cladding</td>
<td>zircaloy-3</td>
<td>Driver fuel peak temperature ($^\circ$C)</td>
<td>820</td>
</tr>
</tbody>
</table>
Figure 1.2: Top view of the TREAT core, permanent reflector, and biological shielding, from Ref. [1].

1.2.2 Irradiation Experiment Vehicle (IEV)

One of the TREAT flexibilities comes from the irradiation experiment vehicles (IEV). In a transient experiment, the specimen is first loaded into the IEV at the Hot Fuel Examination Facility (HFEF) at the INL Materials and Fuels Complex (MFC). The loaded IEV is then transported to TREAT and inserted into the core by replacing one or two TREAT core assemblies. Thus, the specimen is irradiated in an isolated environment in the IEV. If the specimen fails in a transient experiment, the IEV prevents the contamination of the TREAT core. The IEV can be designed to simulate specific environment for the specimen, e.g.,
static fluid/moderator or recirculating coolant system. This allows the experiment to use
essentially any working fluid (water, sodium, helium, etc.) at desired pressures, temperatures
and flow rates [1]. Therefore, TREAT can be used to test different fuels, e.g., light water
reactor fuels and sodium-cooled fast reactor fuels, by using different IEVs (currently available
or designing new ones) without changing the core configuration. In addition, both irradiated
and pre-irradiated fuel specimens can be tested [13].

Different IEVs exist, and the Mark-III sodium loop is one of them. The Mark-III sodium
loop is used in the historic TREAT transient experiments, and it also provides a basis for
the new IEV designs [14]. A schematic of the loop is shown in Fig. 1.3. Two parallel legs
of the loop have a height of 3.5 m and are separated by about 0.1 m [2]. In an experiment,
the loop is first loaded into a container, then, the container replaces one or two TREAT fuel
assemblies to insert into the test hole at the center of the TREAT core, which is shown in
Fig. 1.2. One leg of the loop contains a removable test train to load the specimen. The other
leg has a pump to circulate the sodium coolant. The sodium is circulated to pass through
the specimen in an upward direction, which simulates the coolant environment. Features of
the loop are summarized in Table 1.2.

Up to seven fuel specimens can be loaded into the test train. Each specimen is posi-
tioned in a stainless steel flowtube. At the entrance of each flowtube, a properly-sized orifice
is installed to distribute particular amount of the sodium coolant into the flowtube. Ther-
mocouples are attached to the outer surfaces of each flowtube at the outlet and along the
fuel zone to measure the sodium temperature. To minimize the temperature gradient, the
wall of the flowtube is made with thickness less than 0.5 mm. The flowtube is surrounded
by a shield tube for isolation. The space between the flowtube and the shield tube is filled
with inert gas. If a flowtube fails, the shield tube prevents the debris from damaging the
neighbor flowtubes and the test train.
Figure 1.3: Schematic of the Mark-III sodium loop with three fuel pins loaded, after Ref. [2]. The loop has a capacity of 7 fuel pins.

Table 1.2: Features of the Mark-III sodium loop, after Ref. [14].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design pressure</td>
<td>34.5 MPa at 538 °C</td>
</tr>
<tr>
<td>Test section inlet temperature (pre-transient)</td>
<td>≤ 400 °C</td>
</tr>
<tr>
<td>Volume of sodium</td>
<td>≈ 2 liters</td>
</tr>
<tr>
<td>Mass of sodium</td>
<td>≈ 1.25 kg</td>
</tr>
<tr>
<td>Sodium flow velocity</td>
<td>≤ 7 m/s</td>
</tr>
<tr>
<td>Sodium flow rate</td>
<td>≤ 1.2 liter/s</td>
</tr>
<tr>
<td>Mass of loop</td>
<td>115 kg</td>
</tr>
</tbody>
</table>

1.2.3 Operation Modes

TREAT can be operated in the steady-state and the transient modes. The operating characteristics under different modes are listed in Table 1.3. The steady-state mode has a maximum
thermal power of 120 kW and neutron flux of $4 \times 10^{11}$ cm$^{-2}$s$^{-1}$. The heat generated under this mode can be sufficiently removed by the cooling air. The steady-state mode is mainly used for physics measurements, isotope build-in (e.g., $^{131}$I) for follow-on tests, neutron radiography, and other system checkout operations [3].

The distinctive capability of TREAT is its transients, which can provide neutron flux up to $10^{17}$ cm$^{-2}$s$^{-1}$. Ref. [13] divides the TREAT transients into the temperature limited, shaped, and the extended transients, as shown in Table 1.3. However, Ref. [3] categorizes the transients as the exponential and the shaped transients. The exponential transient has peak flux shape and usually lasts less than a second. The shaped transient offers flat flux shape and can be maintained longer than the exponential transient. The shaped transient is produced by a step insertion of reactivity followed by reactivity insertion or removal at rates required to produce the desired burst shape [3].

Table 1.3: Operating characteristics of TREAT, after Ref. [13]. The nominal pulse duration is the full width at half maximum (FWHM).

<table>
<thead>
<tr>
<th></th>
<th>Temperature limited</th>
<th>Shaped transient</th>
<th>Extended</th>
<th>Steady state</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal pulse duration</td>
<td>&lt; 1 s</td>
<td>seconds</td>
<td>minutes</td>
<td>N.A.</td>
</tr>
<tr>
<td>Max core power (thermal)</td>
<td>19 GW</td>
<td>10 GW</td>
<td>N.A.</td>
<td>120 kW</td>
</tr>
<tr>
<td>Max core energy (MJ)</td>
<td>2900</td>
<td>2900</td>
<td>$\geq 2600$</td>
<td>N.A.</td>
</tr>
<tr>
<td>Max thermal neutron flux (cm$^{-2}$s$^{-1}$)</td>
<td>$1.0 \times 10^{17}$</td>
<td>$1.0 \times 10^{17}$</td>
<td>$1.0 \times 10^{17}$</td>
<td>$4.0 \times 10^{11}$</td>
</tr>
</tbody>
</table>

Duration of the transients is limited by the temperature. A transient is terminated if the peak fuel and clad temperature exceeds 600 °C. In the shaped transients under current core configuration, a step insertion of about 4.6% $\Delta k/k$ can reach the temperature limit of 600 °C, and an insertion of 5.9% $\Delta k/k$ can achieve a temperature of 820 °C [3], which is the driver fuel peak temperature, as shown in Table 1.1. In addition, in the exponential transients, the control rods can be inserted at high drive speed to suspend the transient, i.e., the pulse width is narrowed, before the temperature limit is reached. This mechanism is termed rod-and-temperature-limited excursions [3].
1.2.4 Pulse Narrowing

Upon resumption of TREAT, the LWR fuels, especially the ATFs, will be tested. Behavior of the LWR fuels in the postulated Hot Zero Power Reactivity Initiated Accidents (HZP-RIA) is of interest. An HZP-RIA happens when the control elements (blades, rods, etc.) are withdrawn from an LWR core in the condition that the reactor is preheated to operational inlet temperatures, but not yet producing fission power. A brief nuclear power excursion may happen where rapid fuel pellet thermal expansion could drive cladding failure through mechanical interaction [3].

To simulate the HZP-RIA, the transient pulse width, which is usually measured by full width at half maximum (FWHM), is a critical parameter. Pulses with 30-ms FWHM can create more than doubled peak cladding hoop stress than pulses with 90-ms FWHM [3]. To simulate the HZP-RIAs, the desired pulse width range for pressurized water reactor (PWR) is 25 to 65 ms FWHM, and 45 to 75 ms for boiling water reactor (BWR). However, current FWHM of TREAT pulses is about 100 ms [3], which is too wide for the HZP-RIA testing. Hence, narrowing the TREAT pulses is necessary.

It is under investigation to narrow the TREAT pulse width with increased reactivity insertion (to initiate the pulse) and rapid termination at the end of the pulse (clip) [3]. RELAP5-3D is used to calculate the FWHMs under different reactivity insertions, and the results are shown in Fig. 1.4. In the calculation, the reactor is allowed to response naturally to the reactivity insertion, i.e., the temperature can exceed the 600 °C limit, and no clipping is applied. As the reactivity insertion increases, the FWHM decreases, and the maximum fuel temperature increases. By reducing the total peaking factor from 1.82 to 1.6, which might be achieved via optimizing the core loading, the maximum fuel temperature decreases at the same reactivity insertion. Thus, if the temperature limit is considered, at 600 °C, the total peaking factor of 1.82 allows a reactivity insertion of about 4.46% Δk/k, and the FWHM is about 106 ms. For the total peaking factor of 1.6, the allowed reactivity insertion is approximately 4.85% Δk/k, and the FWHM is 97 ms. Hence, only increasing the reactivity insertion, even under optimized total peaking factor, can not narrow the TREAT pulse width.
to the desired range for the HZP-RIA simulation. Though not effective in narrowing the pulse width, larger reactivity insertion may deposit more energy into the specimen. To allow larger reactivity insertion, numerical core power flattening studies indicate the fuel assembly power can be reduced on the order of about 20% [3], i.e., assuming the maximum core temperature varies linearly with reactivity insertion, at 600°C limit, the reactivity insertion can be increased by a factor of 1.25.

Figure 1.4: FWHM of the TREAT pulse and maximum fuel temperature varies with reactivity insertions, after Ref. [3]. Results under total peaking factors 1.82 and 1.6 are shown.

The clipping techniques are considered to narrow the pulse width further, which consist of increasing the drive speed of the transient rods and a more advanced hypothetical ³He system. Numerical evaluation indicates that, at reactivity insertion of 4.5% ∆k/k, increase the drive speed of the transient rods from the current maximum 140 to 250 inch/s, the FWHM reduces from 95 ms to 77 ms. When the hypothetical ³He system is applied, which represents a reactivity insertion of -5% ∆k/k in 5 ms, the FWHM can be reduced to the desired 46 ms [3]. Hence, the ³He system is more effective than increasing the drive speed of the transient rods. Ongoing efforts focus on realizing the ³He system [3].
1.2.5 In-Core Neutron Detectors

TREAT used the prompt-type Self-Powered Neutron Detectors (SPNDs) to measure the in-core neutron flux [4]. A schematic of the SPNDs is shown in Fig. 1.5, and the details are listed in Table 1.4. The SPNDs consist of the Inconel 600 sheath (collector), the alumina insulator, the emitter (hafnium or gadolinium), and two Inconel leadwires. The sheaths and the emitters have cylindrical shapes. The emitter is embedded in the insulator and is positioned from one end of the tube by 12.7 mm. SPNDs with different emitter lengths were used, where the Hf emitters have lengths of about 40 cm, and the Gd emitters have lengths of 2.413 and 2.852 cm, respectively. To adapt the Hf emitter length comparable to the Gd value, a steel rod was used to shield the emitter region of the Hf SPND, after which the neutron-sensitive section of the Hf SPNDs has length of 3.18 cm [4]. A leadwire connects the emitter to the external electronics. A second leadwire is used to compensate the background signal. This background leadwire differs from the emitter leadwire that it ends in the insulator near (not connects to) the emitter.

Neutrons may be captured in the emitter, and prompt gamma rays are emitted within about $10^{-13}$ s [23]. The gamma rays may interact in the emitter mainly via Compton scattering or the photoelectric effect and generate electrons. Additionally, internal conversion electrons may also be produced [4]. If these electrons have sufficient energy, they may travel to the sheath from the emitter and leave the emitter positively charged. This electron motion can be measured as current in the external circuit, which is the signal.
Table 1.4: Details of the SPNDs used in TREAT, after [4].

<table>
<thead>
<tr>
<th></th>
<th>Hafnium (Hf)</th>
<th>Gadolinium (Gd)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Emitter</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Material</td>
<td>97.5%Hf min., 2.5%Zr max.</td>
<td>99.7%Gd</td>
</tr>
<tr>
<td>Length (cm)</td>
<td>≈ 40</td>
<td>2.413 or 2.852</td>
</tr>
<tr>
<td>Diameter (mm)</td>
<td>0.4572</td>
<td>0.559</td>
</tr>
<tr>
<td>Mass (g) (nominal)</td>
<td>0.873</td>
<td>0.0508</td>
</tr>
<tr>
<td><strong>Leadwire (two each)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Material</td>
<td>Inconel 600</td>
<td></td>
</tr>
<tr>
<td>Diameter (mm)</td>
<td>0.203</td>
<td>0.229</td>
</tr>
<tr>
<td><strong>Sheath</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Material</td>
<td>Inconel 600</td>
<td></td>
</tr>
<tr>
<td>O.D. (mm)</td>
<td>1.372</td>
<td>1.575</td>
</tr>
<tr>
<td>Wall thickness (mm)</td>
<td>0.229</td>
<td>0.279</td>
</tr>
<tr>
<td><strong>Insulation</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Material</td>
<td>Aluminum Oxide</td>
<td></td>
</tr>
<tr>
<td>Purity</td>
<td>99.65%</td>
<td>99.65%</td>
</tr>
<tr>
<td>Compaction</td>
<td>about 70% of theoretical density</td>
<td></td>
</tr>
</tbody>
</table>

The main background of the SPND is the gamma rays from the neutron capture in the core, as opposed to the gamma rays from fission [4]. These gamma rays are proportional to the neutron flux. If the background gamma rays interact in the emitter and eject electrons, the resulted current contributes to signal. However, the background gamma rays may interact within the sheath, and the ejected electrons may travel from the sheath to the leadwire, which produces background potential gradient between the sheath and leadwire. This background potential gradient is compensated by the background leadwire.

Space charge exists in the insulator of the SPND, which is produced by the low-energy electrons. The low-energy electrons entering the insulator may be at thermal equilibrium within the insulator. Due to the charge traps and the insulator’s energy band structure, the electrons spend a finite time (“dwell” time) in the insulator before drifting to the electrode. These electrons in the insulator constitute the space charge [24]. The space charge grows and reaches a quasistatic state, in which the number of electrons entering equals to the number of electrons leaving the insulator. The space charge introduces an electric field, which has
one zero point, or potential peak, in the insulator [25]. The electric field vectors point in opposite directions on the two sides of the potential peak [24], as shown in Fig. 1.6. In other words, for the electrons traveling from the origin electrode (emitter or sheath) to the potential peak, the electric field repels the electrons back to their origin electrode. For the electrons with sufficient kinetic energy to cross the potential peak and traveling from the peak location to the non-origin electrode, the electric field accelerates them. For the SPNDs used in TREAT, the electrons need to have a minimum kinetic energy of about 260 keV to penetrate the space charge, and contribute to the signal [4]. If the kinetic energy is insufficient, the electron is repelled back, and its overall contribution to the signal is zero. Additionally, the space charge is insensitive to the operating temperature of the SPNDs in the TREAT core [4].

![Figure 1.6: Schematic of the force directions on the electrons introduced by the space-charge electric field in the SPNDs.](image)

### 1.2.6 Reactivity and Transient Control Mechanism

Shown in Table 1.5 is the reactivity and control rod characteristics of TREAT. TREAT has a temperature coefficient of $-1.8 \times 10^{-4} \Delta k/k/\degree C$, which is mainly contributed from the graphite in the driver fuel due to a thermal Maxwellian shift with increased leakage [1]. TREAT has 20 control rods with 152.4 cm active absorber length [15]. These 20 control rods
are four Compensation Rods, 8 Control/Shutdown Rods and 8 Transient Rods. Layout of these rods is shown in Fig. 1.7. During transient operation, the Compensation Rods are used at the end of the transient to shut down the reactor, providing excess negative reactivity. The Control/Shutdown Rods are used to establish pre-transient criticality and remain fixed and partially inserted into the core during a transient. The Transient Rods are rapidly withdrawn to initiate transient conditions during transient operation, and can be moved to shape the transient with time. Ref. [3] reports the maximum speed of the transient rods is 140 inch per second. However, Ref. [26] states the transient rods have the maximum speed of 170 inch per second and have a 40-inch stroke, i.e., the transient rods can navigate the full stroke in about 0.24 seconds.

Table 1.5: Reactivity and transient control mechanism characteristics of TREAT, after Ref. [13, 15]. Ref. [13] stats the number of transient rods is one. Ref. [15] reports the number is eight, which is listed here.

<table>
<thead>
<tr>
<th>Temperature coefficient (Δk/k/°C)</th>
<th>–1.8 × 10^{-4}</th>
<th>Moderator</th>
<th>graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of control rods</td>
<td>20</td>
<td>Control rod material</td>
<td>B_{12}C</td>
</tr>
<tr>
<td>Number of transient rods</td>
<td>8 [15]</td>
<td>Transient rod absorbing material</td>
<td>Mild Steel, CP-2 graphite, chrome plating</td>
</tr>
</tbody>
</table>

1.2.7 Hodoscope

The hodoscope is used to monitor the fuel motion in the transient tests. A schematic of the hodoscope is shown in Fig. 1.8. The hodoscope has a thick conical front collimator, a rear collimator with over 300 diverging slots, the lead filter, and the neutron detector arrays to detect the collimated fission neutrons through the respective slots. The real collimator consists of 30 low-carbon steel plates, selection of which over the hydrogenous mixtures is due to the machinability and the attenuation of the gamma rays from the core [11]. The detector slots have approximately 1 inch diameter [6]. Fission neutrons from the specimen can travel through the slotted TREAT hodoscope assemblies, the graphite reflector, and the collimators to be detected. Then, the fuel motion as a function of space and time can be monitored.

While the steel collimator suppresses some gamma rays from the core, it introduces
Figure 1.7: Current layout of the TREAT control rods, after Ref. [3]. T is the transient rods. C is the compensation rod. S is the control/shutdown rod. H represents the slotted hodoscope assembly. TH stands for the test hole.

Figure 1.8: Schematic of the TREAT hodoscope, from Ref. [5].

another source of gamma rays by capturing neutrons from the core and sample. For $^{56}$Fe (with atomic abundance of 91.75% in natural iron), the most-probable gamma rays are 7.6 MeV with intensity of 29±4.94 per 100 neutron captures [27]. The thermal neutron
capture cross section and the resonance integral of $^{56}$Fe are 2.6 and 1.4 barn, respectively. The gamma rays, from the neutron capture in steel and from the core, may further collide via the pair production, Compton scattering, and the photoelectric effect. These capture gammas that arrive the hodoscope fast-neutron detectors constitute a major source of background.

### 1.2.8 Hodoscope Detectors

It is a challenge to design a hodoscope fast-neutron detector that exhibits good performance over the wide power range of TREAT transients (from MW to 19 GW). The original TREAT hodoscope uses the Hornyak button fast-neutron detectors, design of which considers the linearity, count-rate capacity, dead time, gamma-ray rejection, efficiency, time and spatial resolution at 100-MW power [11]. A schematic of the Hornyak button is shown in Fig. 1.9. It consists of a $2.8 \times 15.9 \times 25.4$ mm$^3$ central active rectangular slab and optically coupled half-cylinder PMMA (Lucite) light guides. The slab is a mixture of 5% mass ratio ZnS:Ag in the PMMA.

Fast neutrons primarily interact with the hydrogen in the detector to generate recoil protons. If the recoil protons deposit energy in the suspended scintillating ZnS:Ag particles, light is emitted. The light can then be shuttled to the photomultiplier tube (PMT) connected to the rear end by the light guides to generate detectable pulses. Another mechanism to generate light is the $^{32}$S(n, p)$^{32}$P reaction [28], in which the neutron directly interacts with the sulfur nuclide in ZnS:Ag. The Q value of this reaction is -0.93 MeV, and the microscopic cross section is 0.017 b at 2 MeV. Under ideal conditions, the Hornyak button has an efficiency of about 0.4% for neutrons with energy above 0.1 MeV, with good rejection of about $10^{-8}$ counts per incident gamma ray [11] after applying the pulse-shaping technique [29]. The gamma-ray rejection may be enhanced further by using the passive or active cancellation circuits [30].

The Hornyak buttons lose linearity between count rate and transient power for power levels above 100 MW [11]. At power levels in a few GW, the count rates of the Hornyak buttons are 10 or 20 times greater than the values extrapolated from the readouts at lower
power level, which are mainly caused by the fast neutrons. These large count rates cause channel saturation in the detector responses. The large count rates are verified to be caused by the gamma rays [11]. The gamma rays may generate electrons with velocities larger than the speed of light in the transparent dielectric, e.g., PMMA in the Hornyak button and the photomultiplier glass envelope, via the photoelectric effect, Compton scattering, and pair production [23]. Movement of the high-speed electrons produces the Cherenkov light [31]. This Cherenkov light generates competitive pulses responsible for the excessive noise count rates. To eliminate the nonlinearity caused by the gamma ray flash saturation, a lead filter with thickness ranging from 0.375 in. for 30 MW to 2 in. for 16 GW is placed between the collimator and the detector array [11], as shown in Fig. 1.8.

1.3 Modeling of Novel Neutron Detectors for TREAT

To support future operations of TREAT, alternative hodoscope fast-neutron and in-core thermal-neutron detectors are under development at Kansas State University (KSU). The hodoscope detectors, as alternatives to the Hornyak buttons, are layered and homogenized ZnS(Ag)-PMMA scintillation detectors, and fast-sensitive, microstructured semiconductor
neutron detectors (MSNDs). The in-core detectors considered are the micro-pocket fission detectors (MPFDs), which are alternatives to the SPNDs used in the TREAT core.

The goal of this work is to model and simulate these novel neutron detectors for TREAT to assist development and design. Based on the knowledge of radiation detection, the detectors are designed to have qualitatively good performance for the TREAT applications. Modeling of the detectors can give a quantitative verification of the design by simulating the underlying physics. Simulation is usually cheaper and requires less time than constructing and testing multiple prototypes in the experiments. Numerical evaluation can also calculate quantities that are difficult to measure in experiments. Predictive modeling can be used to optimize the parameters of the detectors. Once optimized detectors are constructed, the numerical and the experimental results can be compared, which contributes to the validation of the simulation codes.

1.3.1 ZnS(Ag)-Based Scintillation Detectors

The proposed hodoscope detectors are designed for good neutron-detection efficiency while rejecting gamma noise using simple pulse-height discrimination, i.e., achieving sufficiently high signal-to-noise (S/N) ratio. The layered and the homogenized ZnS(Ag)-PMMA scintillation detectors are evolutions of the existing Hornyak buttons. The scintillation volume of the layer detector consists of alternating layers of ZnS(Ag) and PMMA. The scintillation volume of the homogenized detectors is like the Hornyak button, i.e., a homogeneous mixture of ZnS(Ag) and PMMA. The scintillation volumes of the new detectors are surrounded by silicon photomultipliers (SiPMs) to collect light. Compared to the Hornyak buttons, the use of SiPMs replaces the light guides and the PMT, which reduces Cherenkov noise.

To evaluate S/N ratios of the hodoscope detectors, the responses to the fast neutrons and the gamma rays in the hodoscope radiation environment are of interest. For the scintillation detectors, the transportations of radiation particles, i.e., neutrons and gamma rays, and light are simulated in Geant4 (for GEometry ANd Tracking) [32]. The Hornyak buttons are modeled to validate the physical models and approximations. The scintillation volumes of
the layered and homogenized variants are modeled to optimize the parameters.

### 1.3.2 Fast-Sensitive MSNDs

The proposed fast-sensitive MSNDs are adapted from the existing, thermal-sensitive design, which has long been developed at KSU, by using fast-sensitive neutron converters. In the fast-sensitive MSNDs, gamma rays may interact within the silicon base, but the strong, gamma-induced Cherenkov noise is eliminated because no transparent dielectric material exists in the devices, and the MSNDs are not scintillation detectors. The fast-sensitive converters considered are actinides and paraffin wax. The actinide MSNDs allow for high, lower-level discriminator (LLD) settings due to the high-energy fission fragments. The major concern is the neutron-detection efficiency that can be achieved with use of actinide reactants. The paraffin wax has a larger macroscopic cross section for fast neutrons than any actinide. Because the recoil protons have less energy than the fission fragments, hydrogenous MSND designs are considered that maximize the energy deposition of the protons in the silicon depletion region to distinguish neutrons from gamma rays.

Fast-sensitive MSNDs are evaluated using Geant4 and MCNP (Monte Carlo N-Particle) [33] for comparison. For the actinide MSNDs, the fission fragment generator (FFG) in Geant4 [34] is used to sample and track the fission fragments in a single run. This feature is more convenient than MCNP, where the energy of the fission fragments is assumed to be deposited locally, i.e., in the volume where the fission reaction happens [35]. To evaluate the actinide MSNDs, the deposited energy outside the fission site, i.e., in the active silicon region, is the tally. For the hydrogenous MSNDs, both codes are used to simulate the neutron responses, and Geant4 is used to evaluate gamma-ray noise.

### 1.3.3 Micro-Pocket Fission Detectors

The MPFDs are gas detectors using the fission reaction to convert in-core neutrons to discernible electric signals. A thin fissile layer is deposited on one side of the chamber. One of the fission fragment pair enters the gas and deposits a few MeV of energy, which distinguishes a
neutron event from other in-core radiations. The deposited energy ionizes electron-ion pairs, and the charge carriers are drifted to respective electrodes under an applied electric field, thereby producing a measurable signal.

To evaluate the dynamic response of MPFDs, a computational routine consisting of the Garfield++ [36], Gmsh [37], Elmer [38], and stopping and range of ions in matter (SRIM) [39] was used. Elmer computes the electric field using the finite-element method based on the meshed geometry generated by Gmsh. SRIM calculates the energy loss tables of the fission fragments in the gas. Garfield++ computes the energy loss of the fission fragment, simulates the drift of electrons in the gas under applied electric field, and calculates the induced signal. The application using Garfield++ is parallelized using hybrid Message Passing Interface (MPI) and OpenMP.

1.4 Organization of the Dissertation

Chapter 2 reviews the common neutron-detection techniques. Chapter 3 reviews the Monte Carlo method and introduces the Geant4 code used to evaluate the neutron detectors. Chapter 4 presents the approximations and physics to evaluate the hodoscope detectors, and the simulated results of the Hornyak buttons. Chapters 5, 6, and 7 models and simulates the Hornyak-button variants, the fast-sensitive MSNDs, and the MPFDs, respectively. Chapter 8 concludes the dissertation and provides the future work.
Neutron Detection Techniques

Neutrons are detected indirectly via signals generated by deposited energy of secondary charge particles. Neutrons are converted to secondary particles through different absorptive or scattering reactions. The secondary particles deposit energy and generate signals via electron-ion pairs in a gas-filled detector, scintillation light in a scintillation detector, and electron-hole pairs in a semiconductor detector. Coupling of neutron converting reaction and signal-forming mechanism creates various neutron detectors for different applications. In this chapter, common neutron detection techniques are reviewed.

2.1 Converting Reactions

To develop neutron detectors for a specific application, the cross section of the converting reaction and the kinetic energy of the secondary charged particles must be considered. The cross section affects the detector’s intrinsic efficiency, and the kinetic energy of the charged particles determines the allowed lower-level discriminator to reject background noise. In this section, these two aspects of common neutron converting reactions are introduced.
2.1.1 Thermal Absorptive Reactions

Three common absorption reactions to detect thermal neutron are compared in Table 2.1.

$^{3}$He gas proportional counters are widely used in neutron scattering science and homeland security applications [40] due to the large thermal neutron cross section (5400 b at 0.025 eV).

Helium-3 gas is produced from the decay of tritium, which is produced by nuclear weapons programs in the U.S. and Russia [40]. Due to the shortage and rising cost of $^{3}$He gas, alternative neutron-detection techniques are sought.

Table 2.1: Comparison of three thermal neutron absorptive reactions, after Ref. [7].

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Charge particles produced</th>
<th>Q value (MeV)</th>
<th>$\sigma$ (b) at 0.025 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{10}$B(n, $\alpha$)$^{7}$Li</td>
<td>$\alpha$, $^{7}$Li</td>
<td>2.78</td>
<td>3840</td>
</tr>
<tr>
<td>$^{6}$Li(n, $\alpha$)$^{3}$H</td>
<td>$\alpha$, $^{3}$H</td>
<td>4.78</td>
<td>937</td>
</tr>
<tr>
<td>$^{3}$He(n, p)$^{3}$H</td>
<td>p, $^{3}$H</td>
<td>0.765</td>
<td>5400</td>
</tr>
</tbody>
</table>

Boron- or lithium-based neutron detectors have been developed as $^{3}$He-replacement techniques. The $^{10}$B reaction has a larger cross section than $^{6}$Li; however, the $^{6}$Li reaction has a larger Q value, which can make discrimination of background radiation easier. One proposed $^{3}$He-replacement technology of relevance to the present work is the microstructured semiconductor neutron detector (MSND) [41], which employs $^{6}$LiF to convert thermal neutrons. The most recent generation of MSNDs (so-called “dual-sided” MSNDs) has exhibited an intrinsic thermal neutron detection efficiency of nearly 70% [42].

2.1.2 Proton-Recoil Reaction

The main scattering reaction to convert fast neutrons is elastic scattering between an incident neutron and a hydrogen nucleus, i.e., a single proton. As shown in Fig. 2.1, a neutron with kinetic energy $E_n$ collides with a proton at rest. The kinetic energy of the recoil proton, $E_p$, for $\theta$ in the laboratory system is

$$E_p = E_n \cos^2 \theta.$$  (2.1)
This scattering process is isotropic in the center-of-mass system for neutron energy up to about 14 MeV, and on average, half of the neutron energy is transferred to the recoil proton. The microscopic cross section of this reaction decreases from approximately 13 b at neutron energy of 0.1 MeV to about 1 b at neutron energy of 10 MeV.

![Kinematics of neutron-proton collision in the laboratory system.](image)

2.1.3 Fission Reactions

Fission reactions are used to convert thermal or fast neutrons, depending on the actinide materials used [43]. $^{235}\text{U}$ has a large fission cross section for thermal neutrons (587 b at 0.025 eV). $^{237}\text{Np}$ exhibits a 0.5-MeV threshold for the fission reaction, and the cross section is about 1 to 2 b for neutron energies between 1 and 10 MeV.

Fission reactions are valuable for use in high-background applications due to the large energy of fission fragments (and, hence, the large energy deposited by those fragments). In the thermal fission of $^{235}\text{U}$, the fission fragments carry away approximately 168 MeV of energy [23], which allows one to use high lower-level discriminator settings.

2.2 Signal-Forming Mechanisms

Secondary charge particles from neutron reactions deposit energy in a detector mainly via Coulomb interactions by ionizing and exciting electrons. Electrons are ionized when they gain sufficient energy from the charge particles to become free particles. If the acquired energy is insufficient, electrons are excited to higher energy states but remain bound to
atoms. The excited electrons may drop to lower energy states with photon emission.

Neutron detectors have different mechanisms to generate signals. The deposited energy liberates electron-ion pairs in a gas-filled detector, generates electron-hole pairs in a semiconductor detector, and produces light in a scintillation detector. In the gas-filled and semiconductor detectors, charge carriers are drifted under an applied bias, which induces current in an external circuit. In a scintillation detector, the scintillation photons may interact within a coupled light sensor, e.g., photomultiplier tube (PMT) or silicon photomultiplier (SiPM) [9], and produce photoelectrons. These photoelectrons are amplified by the light sensor to generate a measurable signal.

2.2.1 Gas-Filled Detectors

The response of a gas-filled detector to incident radiation depends critically on the relationship between applied voltage and collected charges, which is shown in Fig. 2.2. When a charged particle enters the gas, it deposits energy and ionizes electron-ion pairs along its path. For many commonly used gases, the energy $w$ required to create an electron-ion pair is between 20 and 40 eV (e.g., $w$ for Ar is 27 eV) [44]. The primary electron-ion pairs are drifted under applied electric field. In the recombination region, the electric field is not strong, and ionized electrons may recombine with ions; hence, little or no signal is formed. No detectors are operated in this region.

As the applied voltage is increased to the ionization regime, recombination is effectively eliminated, and the electron-ion pairs are drifted apart completely. The collected charges are proportional to the deposited energy. Hence, the total amount of charge produced by incident $\alpha$, $\beta$, and $\gamma$ particles differ. In addition, the primary ionized electrons are not accelerated by the electric field sufficiently to produce secondary ionizations. Thus, the induced current is small. Detectors operated in this region are called ion chambers, and represent the gas detectors of interest for in-core applications at TREAT and elsewhere in this work.

However, further increasing the applied voltage leads to two additional characteristics responses, which are described here for completeness. When the applied voltage enters
the proportional region, electrons gain sufficient kinetic energy from the electric field to produce secondary ionizations and excitations. This effect is called *impact ionization* \[23\], and *gas multiplication* appears. The measured current is stronger than ion chambers and still proportional to the original deposit energy. Detectors operated in this region are named *proportional counters*.

With applied voltage in the Geiger-Muller region, gas multiplication is tremendous. Regardless of the initial deposited energy by the charged particle, the output pulse heights are essentially the same (i.e., to within statistics). The pulse heights are determined by the detector configuration, and incident particles are not distinguishable. Detectors operated in this region are termed *Geiger-Muller (GM) counters*.

When applied voltage increases beyond the GM region, continuous discharge occurs. No detectors are operated in this region.

![Figure 2.2: The collected charges vary with applied voltage in the gas-filled detectors irradiated by \(\alpha\), \(\beta\), and \(\gamma\) particles, after Ref. \[7\].](image)

**Figure 2.2:** The collected charges vary with applied voltage in the gas-filled detectors irradiated by \(\alpha\), \(\beta\), and \(\gamma\) particles, after Ref. \[7\].
Ion chambers can be operated in pulse mode or current mode. In pulse mode, the induced current is integrated by an external circuit to produce a voltage potential. The voltage is measured to indicate a single radiation event. Then, the circuit is discharged and reset for next radiation event. Pulse mode is generally not suitable for high radiation environment. When the circuit is integrating or discharging current, if a new radiation event happens, it can not be recorded. The period during which a detector cannot respond is called the dead time. Hence, radiation events during dead time need to be avoided by decreasing the dead time or by reducing the neutron-converting reaction rate.

For high radiation fields, current-mode operation is more often used, where the induced current is measured by an ammeter. The measured current indicates the ionization rate from many radiation events in the detector, and a single radiation event is not revealed.

Charge collection within an ion chamber depends on the applied voltage and the associated electric field. To calculate the electric field, the electric potential \( \psi \) (V) has to be determined, which follows the Poisson equation, i.e.,

\[
\nabla^2 \psi = -\rho/\epsilon, \tag{2.2}
\]

where \( \rho \) is the volumetric charge density (C/cm\(^3\)), and \( \epsilon \) is the permittivity of the gas (F/cm). Equation (2.2) can be solved subject to appropriate boundary conditions based on the applied bias at the electrodes. Then, the electric field \( \xi \) (V/cm) is

\[
\xi = -\nabla \psi. \tag{2.3}
\]

Subject to this electric field, the charge carrier drift speed \( v_d \) (cm/s) is

\[
v_d = \mu \xi. \tag{2.4}
\]

where \( \mu \) is the mobility (cm\(^2\) V\(^{-1}\) s\(^{-1}\)). Mobility is inversely proportional to gas pressure. In
calculations, mobility is prepared, e.g., by the MAGBOLTZ program [45], to compute the drift velocity.

Another component of the carrier movement is diffusion, which describes the behavior of a charge cloud. The diffusion rate can be expressed as

\[
\frac{\partial \rho(r,t)}{\partial t} = D \nabla^2 \rho(r,t),
\]  

(2.5)

where \( D \) is the diffusion coefficient (cm\(^2\)/s). The diffusion coefficient relates to the mobility as [10]

\[
\frac{D}{\mu} = \frac{kT}{q_e},
\]  

(2.6)

where \( k \) is Boltzmann’s constant, \( T \) is temperature in K, and \( q_e \) is elementary charge. Unlike the deterministic drift velocity, the velocity due to diffusion \( v_D \) of a charge carrier in the cloud is stochastic. With sampled \( v_D \), the actual velocity \( v \) is a vector sum of the drift and diffusion components, i.e.,

\[
v = v_d + v_D.
\]  

(2.7)

In a Monte Carlo simulation, the distance traveled in a step due to diffusion is sampled based on the calculated drift distance; this sampling process is described more thoroughly in Chapter 7.

Charge carrier motion induces a current in the external circuit. This induced current can be determined easily using the Shockley-Ramo theorem, which defines

\[
\mathbf{i}(t) = -Q \mathbf{v} \cdot \mathbf{E}_w(r_Q),
\]  

(2.8)

where \( Q \) is the charge, and \( \mathbf{E}_w \) is the weighting electric field at the charge location \( r_Q \). The weighting electric field can be calculated by applying unity voltage at the anode. While the induced current can also be computed by the Green’s reciprocation theorem [10], the Shockley-Ramo theorem is easier to use and is implemented in the Garfield++ code [36].

Because the electron mass is thousands times less than that of an ion, under the same
electric field, electrons move much faster than ions. Hence, pulses of ion chambers are usually truncated once all electrons are collected for the quickest response, i.e., the resulting pulses are almost entirely from electron motion.

Ion chambers using fission reaction to convert neutrons are called fission chambers. Fission chambers are frequently used inside nuclear reactor cores. Considering the large amount of energy deposited by fission fragments in the gas, fission chambers have the potential to be operated in pulse mode and to isolate neutron signals from other intense radiations in the core, e.g., gamma rays, by pulse height discrimination. However, pulse mode is not intrinsically suitable for intense in-core radiation due to dead time. To circumvent this issue, in-core fission chambers are designed to collect ionized electrons rapidly for small dead time that accommodates the in-core radiation. One candidate technology is the micro-pocket fission chambers [46] developed at Kansas State University, detailed models of which are developed and described in Chapter 7.

2.2.2 Inorganic Scintillation Detectors

A scintillation detector consists of the scintillator and the photon-detection device. Scintillators can be categorized as inorganic, organic, or gaseous. Because the ZnS:Ag-based scintillation detectors considered in this work are the inorganic type, a brief overview of the associated scintillation mechanism is warranted. The scintillation light is weak, and, thus, it is necessary to couple a scintillator with a photon-detection device to convert and amplify the light to measurable electrical signal. Commonly-used photon-detection devices are the traditional photomultiplier tube (PMT) and the more recent silicon photomultiplier (SiPM). For performance, the response of the light sensor should match the emission spectrum of the scintillator.

Inorganic Scintillation Mechanism

When an inorganic scintillator is irradiated, the ionizing particles deposit energy in it and liberate electron-hole pairs. Energy from relaxation and thermalization of charge carriers is
released as intrinsic photons, or transfers to activator and causes extrinsic photon emission [8]. The electron-hole pairs can be generated in several ways. The primary electron-hole pairs are excited directly by the ionizing particles. The energetic primary electrons travel through the scintillator lattice and liberate secondary electron-hole pairs. Furthermore, when an outer-shell electron fills the hole, a characteristic X ray or an Auger electron is emitted with energy equals to the difference of the binding energy between the outer-electron and the inner-hole orbitals. The subsequent emissions can be reabsorbed, and more electron-hole pairs are liberated.

The electron transition and the associated scintillation mechanism can be explained by energy band theory, as shown in Fig. 2.3. The electrons of an atom exist in discrete energy states. When \( N \) identical atoms are arranged to form a crystal, each energy state of an atom splits into \( N \) states because, according to the Pauli exclusion principle, two electrons cannot have the same quantum number in a molecule. Because the atomic density in a solid is about \( 10^{22} \text{ cm}^{-3} \), the energy states from splitting are closely spaced in energy (with gap in the order of \( 10^{-22} \text{ eV} \)) and can be considered as quasi-continuum [10], i.e., an energy band.

The uppermost allowed band filled with electrons is the valence band, below which is the tight-bound band. Above the valence band are the conduction and upper bands, which are empty in a ground-state crystal. An electron can be excited from the valence or the lower tight-bound band to the conduction or upper band and leave a hole in the original band, which forms a free electron-hole pair. Then, the energetic electron loses energy, e.g., via Coulombic interactions during traveling through the lattice, and drops back to the lower edge of the conduction band \( E_c \). If the energy an electron gained is insufficient, the electron is liberated to the exciton band instead of the conduction (or upper) band, where the upper edge of the exciton band is \( E_c \). In this case, the electron still binds to the respective hole, i.e., this pair diffuses together, and such pair is called an exciton. The energy gap of an exciton is slightly smaller than the band gap energy \( E_g \), which is the difference between the upper edge of the valence band \( E_v \) and \( E_c \), as shown in Fig. 2.3. When an electron (from the upper, conduction, or exciton bands) falls back to \( E_v \), photons are emitted. The photons that have energy \( E_g \) are reabsorbed by the scintillator. Therefore, the scintillator is usually
opaque to its own light. This process is the intrinsic photon emission.

To avoid reabsorption, activator is added to the scintillator, which creates energy states in the band gap. As shown in Fig. 2.3, $E_{t0}$ is the ground state of the activator, and $E_{t1}$ and $E_{t2}$ are the excited states. A raised electron may fall into the excited states (e.g., $E_{t1}$ and $E_{t2}$). When the electron deexcites to $E_{t0}$, sub-band-gap photon is emitted and not absorbed by the scintillator. This photon emission is described as extrinsic, i.e., the photons are from the added activator atoms. The extrinsic photons usually have less energy, or longer wavelength, than the intrinsic ones.

![Figure 2.3: Intrinsic and extrinsic scintillation mechanisms, after Ref. [8]. Abbreviations: $E_c$, conduction band edge; $E_v$, valence band edge; $E_{t0}$, activator ground state; $E_{t1}$ and $E_{t2}$, activator excited states.](image)

Only a fraction of the deposited energy is transferred to the extrinsic photons. Part of the energy ends in thermal form without light emission. If the electrons are excited by gamma rays, the wavelength at the peak of the incident gamma-ray spectrum differs from that of the light emission spectrum. This wavelength difference is the Stokes shift [8]. The fraction of the
dissipated energy that is converted to the scintillation response is defined as the scintillation efficiency. Among known inorganic scintillators, NaI:Tl has the highest scintillation efficiency of about 12% [7]. The scintillation efficiencies of other inorganic scintillators are reported as fractions respective to the value of NaI:Tl.

**Photon-Detection Devices**

The scintillation light is week, and it has to be amplified by the photon-detection device for a measurable signal. Two important parameters of a photon-detection device are the quantum efficiency and the photo-detection efficiency (PDE). The quantum efficiency is the number of photoelectrons emitted from the photocathode per incident photon, and the PDE is the overall efficiency of detecting an incident photon.

The traditional light sensor used with scintillators is the photomultiplier tube (PMT), the operational principles of which are shown in Fig. 2.4. The scintillation photons may interact within the photocathode and produce photoelectrons. Guided by the steering voltage, the photoelectrons strike the first dynode in the vacuum tube of the PMT and liberate more electrons. The new electrons undergo the same process in the following dynodes. In the end, the large number of electrons generate measurable electrical signal at the anode.

The total charge produced at the anode is

\[ Q = qN_0 \prod_{i=1}^{M} \bar{g}_i, \]

where \( q \) is the charge of an electron, \( N_0 \) is the number of initial photoelectron, \( M \) is the number of dynodes, and \( \bar{g}_i \) is the average gain of a dynode. The typical total gain (i.e., \( \prod_{i=1}^{M} \bar{g}_i \)) of contemporary PMTs ranges from \( 10^5 \) to \( 10^7 \) [47]. The usual peak quantum efficiency of PMT is about 25%, and higher value of about 35-40% has been reported [48].

Another photon-detection device is the SiPM. A SiPM integrates about 500-4000 tiny avalanche photodiodes (APDs) per mm\(^2\) on a substrate, which forms a macroscopic unit of about 6 mm × 6 mm (or less) [8, 9]. Each APD is connected to a load resistor in series. The
Figure 2.4: A scintillation detector consists of coupled scintillator and PMT, after Ref. [8].

\[
V_a = V - I \times R, \tag{2.10}
\]

where \( V \) is the applied reverse bias voltage across the APD and the resistor, \( I \) is the current, and \( R \) is the resistance of the load resistor. The reverse bias voltage is usually 10-20\% larger than the breakdown value [49], and it operates each APD in the Geiger mode. In this mode, when a photoelectron is produced in an APD, the applied voltage accelerates it to sufficient energy to create electron avalanche via collisions with bound electrons. From a macroscopic view, the semiconductor conducts current. This phenomenon is termed avalanche breakdown. When the current increases to certain limit, e.g., 10 \( \mu \)A [9], due to the series-connected resistor, the voltage across the APD drops below the breakdown value (as shown in Eq. (2.10)), then, the avalanche is quenched. The signals of the independent APDs are summed to measure the light flux.

The gain of an APD is in the level of 10^6 [9]. The quantum efficiency of an SiPM is close to 100\%. However, its PDE deteriorates because 1) the detector surface has insensitive region; 2) only a fraction of photoelectrons can initiate a Geiger discharge; and 3) the pixel needs recovery time [9]. In general, the PDE of SiPM is better than PMT. Shown in Fig. 2.5 is a comparison between the PDEs of SiPMs to the quantum efficiency of a commercial PMT, where the peaks are comparable. Furthermore, as of 2018, the blue-sensitive SiPM has achieved a PDE of 60\% around 400 nm [50]. Another attractive feature of SiPMs is its
insensitivity to magnetic field, and hence, it is preferred over PMT in applications where magnetic field exists, e.g., medical imaging and high-energy physics experiments [50].

For the TREAT hodoscope, the background gamma rays generate strong Cherenkov noise in the PMT connected to the Hornyak button. Such noise can be avoided if SiPM were instead used. Though the gamma rays may still interact with silicon ($Z = 14$), this noise is relatively easy to discriminate by pulse height.

![Figure 2.5: Comparison of SiPM PDEs to quantum efficient of PMTs, after Ref. [9].](image)

2.2.3 Semiconductor Detectors

The electrical conductivity of a semiconductor increases with temperature, which distinguishes it from conductors and insulators. The energy gap of a semiconductor is small. For example, at room temperature, the gap is 1.12 eV for silicon [7], and, hence, electrons can gain thermal energy to jump from the valence band to the conduction band and leave a hole in the valence band. As temperature increases, more electrons are excited, which improves electrical conductivity. Besides the elevated electrons due to temperature, extra electrons
are liberated when radiation energy is dissipated, which is termed charge carrier injection [10]. The excess charge carriers can be measured to reflect the deposited energy by radiation, which is the basis of semiconductor detectors.

Semiconductor neutron detectors can be constructed with micro structures to achieve high efficiency. One notable example is the dual-sided microstructured semiconductor neutron detector (DS-MSND), which has achieved intrinsic thermal-neutron detection efficiency of 69.2% [42]. As an evolution, the fast-sensitive MSND is considered for the TREAT hodoscope in this work.

Recombination

The excited electrons may directly fall back to the valence band from the conduction band and recombine with the holes, which is the radiative electron recombination. In practice, the radiative electron recombination is rare, and the trap-assisted, or the Shockley-Read-Hall (SRH) recombination is more probable [10]. In a semiconductor, defects and impurities, e.g., n- and p-type dopings, create trap states in the gap. The charge carriers that transit through the gap may be captured by the trap states, and the trapped carriers may also be re-emitted, e.g., electrons to the conduction band and holes to the valence band. The SRH recombination affects the time during which an electron stays in the conduction band (or a hole in the valence band), the average of which is the electron lifetime \( \tau_n \) (or the hole lifetime \( \tau_p \)).

Energy Resolution

Semiconductor detectors have good energy resolution and are frequently used in spectroscopy measurement. The energy resolution \( R \) is defined as [7]

\[
R = \frac{\Gamma}{E_0} \propto \sqrt{\omega F},
\]

(2.11)

where \( \Gamma \) is the full width at half maximum (FWHM) of a detector pulse from dissipated energy \( E_0 \), \( \omega \) is the average energy needed to produce a pair of charge carriers, and \( F \) is the
*fano factor*, defined as

\[ F = \frac{\sigma^2_N}{N}, \]

where \( N \) is the number of charge-carrier pairs produced, and \( \sigma_N \) is the standard deviation of \( N \).

For a semiconductor, an energy of 3 to 5 eV is required to create an electron-hole pair. As a comparison, for a gas-filled counter, it takes about 25 to 40 eV to create an electron-ion pair, and for a scintillator-PMT detector, 100 eV to 1 keV is needed to produce a photoelectron. Hence, more charge carriers are produced in semiconductor detector per deposited energy, which decreases the statistical error and provides better energy resolution.

**pn junction**

Semiconductors are doped with donor or acceptor atoms to increase electrical conductivity. A donor atom has more than four valence electrons, while an acceptor atom has fewer than four electrons. Semiconductors with donor (acceptor) atoms are *n*-type (*p*-type), and the conductivity is mainly due to electrons (holes). The doping effects can be explained by the energy band theory, as shown in Fig. 2.6. The excess electron of a donor sits in an energy level close to the conduction band. A small amount of energy, e.g., thermal energy at room temperature, can elevate it into the conduction band. The acceptor atom creates an energy level close to the valence band. An electron of the semiconductor atom can move to this level with a small amount of energy, and a hole is created in the valence band. In both cases, more charge carriers are produced per deposited energy than the un-doped semiconductor, and the conductivity increases.

Semiconductor detectors can be designed as *pn*-junction diodes, *pin*-junction diodes, Schottky diodes, resistive detectors, and photoconductors, but the emphasis here is on the *pn* junction, which is used for the present generation of MSNDs [51]. A *pn* junction is usually formed by transforming one end of a certain type semiconductor into another one, e.g., the MSNDs are fabricated by diffusing *p*-type contacts into *n*-type silicon [51].

A *n*- or *p*-type semiconductor is neutral. When a *pn* junction is formed, electrons dif-
fuse from the high-concentration $n$-type to the $p$-type side, and holes move in the opposite direction. The heterogeneous electron and hole concentrations, i.e., space charge, create an internal electric field, which acts against the diffusing process. When diffusion is compensated by drift due to the electric field, equilibrium is established. The width of the space-charge region is called the depletion or active region (usually, it is expanded by an external reverse bias). If electron-hole pairs are generated by radiation in this region, the charge carriers are swept away under the electric field, which is measured as a signal.

The width of the space-charge region can be derived from the Poisson equation (Eq. (2.2)) [10]. In one-dimension, it becomes (assuming uniform permittivity)

$$\frac{d^2 \psi}{dx^2} = -\frac{\rho(x)}{\epsilon} = \frac{q_e}{\epsilon}(N_A^- + n - N_D^+ - p). \quad (2.13)$$

$N_A^-$ and $N_D^+$ are charge densities introduced by acceptor and donor concentrations, respectively. An acceptor atom is like a negative ion when it receives an extra electron, and a donor
atom loses an electron and becomes an ion. Without radiation, \( n \) and \( p \) are electron and hole concentrations introduced by temperature, diffusion, and drift. At \( n \)-type side, the charge density is mainly dominated by the doping concentration \( N_D^+ \), and at 300K, \( N_D^+ \approx N_D \), i.e., all the donors lose electrons and become ions. The same approximation applies to the \( p \)-type side. Hence,

\[
\frac{d^2 \psi}{dx^2} \approx \begin{cases} 
-q_e N_D / \epsilon, & 0 \approx x \approx x_n; \\
q_e N_A / \epsilon, & x_p \approx x \approx 0,
\end{cases}
\]  

(2.14)

where a schematic is shown in Fig. 2.7. Here, \( x_p \) is the coordinate of the left edge of the \( p \)-type side with a negative value.

\[\text{Figure 2.7: Distribution of the electric field in the depletion region of the } \text{pn junction, after Ref. [10].}\]

The generated electric field \( \xi \) can be computed by

\[\xi = -\nabla \psi = - \int dx \frac{d^2 \psi}{dx^2} .\]  

(2.15)

In the \( n \)-type side,

\[\xi(x) = - \int dx \left( -\frac{q_e N_D}{\epsilon} \right) = \frac{q_e N_D x}{\epsilon} + C_1 .\]  

(2.16)

Similarly, in the \( p \)-type side,

\[\xi(x) = - \int dx \left( \frac{q_e N_A}{\epsilon} \right) = -\frac{q_e N_A x}{\epsilon} + C_2 .\]  

(2.17)
\( C_1 \) and \( C_2 \) can be determined by the boundary conditions that \( \xi(x_n) = \xi(x_p) = 0 \). Then,

\[
\xi(x) = \begin{cases} 
q_e N_D (x - x_n) / \epsilon, & 0 \simeq x \simeq x_n; \\
q_e N_A (x_p - x) / \epsilon, & x_p \simeq x \simeq 0. 
\end{cases}
\]  

(2.18)

The electric fields in both regions are negative, which corresponds to the direction pointing from the \( n \)-type end to the \( p \)-type end. At \( x = 0 \), the electric field is continuous, which requires

\[- N_D x_n = N_A x_p, \]

(2.19)

i.e., the space-charge width in one side is inversely proportional to its doping concentration. In addition, the maximum magnitude of the electric field is at \( x = 0 \), i.e.,

\[\xi_{\text{max}} = - \frac{q_e N_D x_n}{\epsilon} = \frac{q_e N_A x_p}{\epsilon}. \]

(2.20)

The potential difference across the depletion region is

\[
\Delta \psi = - \int_{x_p}^{x_n} dx \xi(x) \\
= - \int_{x_p}^{0} q_e N_A (x_p - x) dx - \int_{0}^{x_n} dx q_e N_D (x - x_n) \\
= \frac{q_e}{2\epsilon} (N_A x_p^2 + N_D x_n^2). 
\]

(2.21)

Based on Eq. (2.19),

\[
N_A x_p^2 = \frac{N_D^2 x_n^2}{N_A} \\
N_D x_n^2 = \frac{N_A^2 x_p^2}{N_D}. 
\]

(2.22)
Upon substitution of Eq. (2.22) into Eq. (2.21), the widths $x_n$ and $x_p$ can be expressed as

$$x_n = \sqrt{\frac{2e\Delta\psi}{q_e}} \frac{N_A}{N_D(N_D + N_A)}$$

$$x_p = -\sqrt{\frac{2e\Delta\psi}{q_e}} \frac{N_D}{N_A(N_D + N_A)}.$$  \hspace{1cm} (2.23)

Then, the total width $W$ is

$$W = x_n - x_p = \sqrt{\frac{2e\Delta\psi}{q_e} \frac{N_A + N_D}{N_A N_D}}.$$ \hspace{1cm} (2.24)

If an external reverse bias voltage $V$ is applied, which is usually much larger than the built-in potential difference $\Delta\psi$, the total width can be approximated as

$$W = \sqrt{\frac{2e(\Delta\psi + V)}{q_e} \frac{N_A + N_D}{N_A N_D}} \approx \sqrt{\frac{2eV}{q_e} \frac{N_A + N_D}{N_A N_D}}.$$ \hspace{1cm} (2.25)

If the doping of one side is much larger than the other, the width can be further simplified to

$$W \approx \sqrt{\frac{2eV}{q_e N_l}},$$ \hspace{1cm} (2.26)

where $N_l$ is the smaller doping concentration. When energy is dissipated in this depletion region, electron-hole pairs are produced and drifted under the bias. The resulting charge carriers are extracted from the semiconductor through an ohmic contact. Then, the signal is amplified, measured, and recorded by counting electronics.

In a semiconductor detector, the electron drift velocity is about two to three times that of a hole \cite{7}. In addition, the depletion region is usually in mm. Thus, both carriers can be collected in the order of $10^{-7}$ s. This feature is different from a gas-filled ionization chamber, in which the drift velocity of electrons is thousands of times larger than the ion velocity. Therefore, in a gas chamber, pulses are truncated when electrons are collected.
2.3 Summary

In this chapter, common neutron converting reactions and the signal-forming mechanisms of gas-filled, scintillation, and semiconductor neutron detectors are reviewed, which cover fundamental physics of the neutron detectors evaluated in this work. The Hornyak buttons and the variants are scintillation, fast-neutron detectors mainly based on the proton-recoil reaction. The fast-sensitive MSNDs convert fast neutrons by the proton-recoil or the fission reaction. The MPFDs are gas-filled fission chambers. In the next chapter, the Monte Carlo simulation to evaluate the neutron detectors will be presented.
Monte Carlo Simulation

The Monte Carlo method has been widely used to simulate radiation transport, and different
codes have been developed, e.g., GEometry ANd Tracking (Geant4) and Monte Carlo N-
Particle (MCNP). In this chapter, the theoretical foundation of the Monte Carlo method
and the general flow of a Monte Carlo simulation of particle transport are presented. Then,
a typical structure used in this work to build Geant4 applications is introduced. Following
this structure, an example problem is modeled in Geant4 and MCNP to compare the inputs.
In addition, a summary is given of the optical physics models in Geant4, which are needed
to simulate scintillation detectors.

3.1 Monte Carlo Basis

The theoretical foundations of the Monte Carlo method are the law of large numbers and the
central limit theorem. The law of large numbers states that, with infinite trials, the sampled
frequency reveals the underlying probability distribution, and the sample mean ($\bar{z}$) equals
the true (population) value $\langle z \rangle$. Consider a definite integral, which can be defined formally
as the sum

$$\frac{1}{N} \sum_{i=1}^{N} z(x_i) \equiv \bar{z} \xrightarrow{N \to \infty} \langle z \rangle \equiv \int_{a}^{b} z(x) f(x) dx,$$  \hspace{1cm} (3.1)
provided that the mean exists, the variance is bounded, and \( x_i \) are sampled from the probability distribution function (PDF) \( f(x) \). It is, of course, impossible to simulate an infinite number of trials. When a large number of histories are simulated, the statistical error is given by the central limit theorem, which states that \( \frac{|\bar{z} - \langle z \rangle|}{\sigma(z)/\sqrt{N}} \) follows a unit normal distribution, i.e.,

\[
\text{Prob}\left\{ \frac{|\bar{z} - \langle z \rangle|}{\sigma(z)/\sqrt{N}} \leq \lambda \right\} = \frac{1}{\sqrt{2\pi}} \int_{-\lambda}^{\lambda} e^{-u^2/2} \, du ,
\]

(3.2)

where \( \sigma(z) \) is the true standard deviation of \( z \). Typically, the true standard deviation \( \sigma(z) \) is approximated by the standard deviation of the sample, \( s(z) \), defined as

\[
s(z) = \sqrt{\frac{N}{N-1} (\bar{z}^2 - \bar{z}^2)} ,
\]

(3.3)

which converts Eq. (3.2) into

\[
\text{Prob}\{ \bar{z} - \lambda \frac{s(z)}{\sqrt{N}} \leq \langle z \rangle \leq \bar{z} + \lambda \frac{s(z)}{\sqrt{N}} \} \simeq \frac{1}{\sqrt{2\pi}} \int_{-\lambda}^{\lambda} e^{-u^2/2} \, du .
\]

(3.4)

Equation 3.4 implies the standard deviation of the sample is inverse proportional to square root of the number of histories, i.e.,

\[
s(z) \propto \frac{1}{\sqrt{N}} .
\]

(3.5)

In addition, \( \frac{s(z)}{\sqrt{N}} \) is the standard error of the sample mean \( \bar{z} \), i.e.,

\[
s(\bar{z}) \equiv \frac{s(z)}{\sqrt{N}} = \sqrt{\frac{\bar{z}^2 - \bar{z}^2}{N-1}} .
\]

(3.6)

The right hand side of Eq. (3.4) is the confidence coefficient, and its truncated percentage form is the confidence limit. The parameter \( \lambda \) defines the width of the distribution in number of standard deviations of the sample mean, i.e., \( s(\bar{z}) \). For \( \lambda = 1, 2, \) and 4, the confidence limits are 68.27\%, 95.45\%, and 99.99\%, respectively, which means, e.g., for \( \lambda = 1 \), the true value \( \langle z \rangle \) has a probability of 68.27\% to fall into the interval of \([\bar{z} - s(\bar{z}), \bar{z} + s(\bar{z})]\).
3.2 Flow of Monte Carlo Simulation

A particle interacts with a material region following different probability distributions, which are used to sample parameters in a Monte Carlo simulation that include the distance traveled before a next collision, the nuclide with which an interaction occurs at a collision site, and the specific reaction that occurs. While the behaviors of individual particles vary, according to the law of large numbers, the average tally from many individual particles (called “histories”) converges to the true average behavior.

In a continuous-energy, Monte Carlo simulation\footnote{The sampling of multi-group simulation is slightly different and not covered here.}, particles are tracked from birth to death, during which the tallies are accumulated. The simulation starts with sampling the initial condition, e.g., energy, position, and direction, of the source particle from user input. Then, the distance to the next collision is sampled from the total macroscopic cross section of the material $\Sigma_t$ by

$$d = -\frac{\ln \xi}{\Sigma_t},$$

(3.7)

where $\xi$ is a pseudorandom number sampled from uniform distribution on $[0,1)$. If the sampled distance exceeds the distance to the global boundary, i.e., the particle streams out of the volume of interest, the particle is killed. If the passed boundary is not global, the particle is moved to the boundary and placed inside the neighbor volume, and a new distance is sampled. If the distance is within the same volume, a collision occurs. Whether the particle passes the boundary or collides, the above process is a Monte Carlo step.

The collision nuclide is sampled based on the discrete probability distribution

$$P(i) = \frac{\Sigma_{t,i}}{\Sigma_t},$$

(3.8)

where $\Sigma_{t,i}$ is the macroscopic cross section of nuclide $i$. The undergoing reaction with the nuclide is likewise sampled from

$$P(j) = \frac{\sigma_j}{\sigma_t},$$

(3.9)
where $\sigma_j$ and $\sigma_t$ are the microscopic cross sections for reaction $j$ and the nuclide. If scattering occurs, the outgoing angle and energy of the particle are sampled from corresponding distributions, and the process from Eq. (3.7) is repeated. If the particle is absorbed, it is killed. If secondary particles are generated, e.g., fission and $(n,xn)$ reactions, they are banked for later tracking. The cross sections and algorithms to simulate different reactions are usually stored in a specific data format, e.g., the ACE data produced by NJOY are used by MCNP, Serpent, and OpenMC, and the G4NDL neutron data library is used in Geant4. During the tracking, the tally and square of the tally are accumulated to compute the mean (Eq. (3.1)) and variance (Eq. (3.3)). When the tracking of particles is completed, i.e., the particles are absorbed or stream out of the global boundary, the simulation is finished.

3.3 Overview of Geant4

Geant4 is a toolkit to simulate passage of particles through matter [32]. It is open-source and written in the object-oriented programming language C++. The code was first released for modeling of high-energy physics (HEP) experiments in December 1998 [52], and now, it has been extended to applications in medical physics, nuclear engineering, and reactor physics [53].

The accuracy of Geant4 has been improved with subsequent releases. Specific improvements include an update of the neutron data library and the incorporation of thermal elastic scattering (i.e., $S(\alpha, \beta)$) laws. In previous versions, the Geant4 neutron data library (G4NDL) was based on 9 different databases, but since version 9.5, G4NDL is solely built on the Evaluated Nuclear Data Files (ENDF/B-VI and VII) [34]. In addition, the $S(\alpha, \beta)$ data matrix has been adopted since version 8.2 [54] to provide the double-differential cross section of thermal-neutron scattering, i.e., the probability that a neutron scatters into certain final-state energy and angle.

Geant4 has several useful features. It can simulate optical physics, which are needed to evaluate scintillation detectors. It has the fission fragment generator (FFG) to sample and to track fission fragments [34]. In contrast, an approximation incorporated in MCNP
is to assume the fission energy is deposited at the location of the fission event. The FFG simplifies the evaluation of fission-based detectors, where the deposited energy by fission fragments outside the fission volume is of interest.

A Geant4 model can be built directly with C++ code (the "batch mode") or by using the more convenient macro commands in a script-like input. Macro commands are text-format equivalents to the corresponding C++ features. For instance, the macro command, `/run/beamOn`, is equivalent to the `BeamOn` function defined in the Geant4 run manager class. Different macro commands for important Geant4 setting functions have been predefined via the “intercoms” category of Geant4 source code. If the functions without corresponding macro commands are needed (which is common), the Geant4 application can be developed using a combination of C++ code and macro commands. In such a case, the macro commands are listed in a text file passed to Geant4 executable via the command line. The Geant4 applications in this work were developed in batch mode assisted by macro files.

### 3.4 Code Structure of Geant4 Application

The code structure of Geant4 applications developed in this work is shown in Fig. 3.1, together with corresponding MCNP input cards. A Geant4 simulation consists of three mandatory user initialization classes: the detector construction class, the physics list class, and the action initialization class. The action initialization class coordinates the mandatory primary generator class and the optional user run, event, and step action classes. The customized classes inherit from respective base classes defined in Geant4 source to communicate with the kernel via defined functions.

#### 3.4.1 Detector Construction

A customized detector construction class inherits from the `G4VUserDetectorConstruction` class to define geometry and material in the `Construct` function. This class is equivalent to

---

2 Names of the Geant4 source classes are with prefix G4.
the surface, cell, and material cards in MCNP. The Geant4 geometry is constructed directly
via volumes, which differs from the MCNP syntax that surfaces are first defined, and volumes
are described using surrounding surfaces. The geometry construction in Geant4 starts with
defining a world volume, whose boundary and coordinate system are global. Then, daughter
volumes are defined and put into the world volume. A daughter volume may contain the
“grand-daughter” volumes, and this hierarchy continues as necessary.

A volume is defined via solid, logical volume, and physical volume classes. The solid
classes implement the Constructive Solid Geometry (CSG) to model different shapes. A
solid is filled with material to construct the logical volume. The logical volume has its
own coordinate system, and it is placed into the coordinate system of its mother logical
volume via the definition of a physical volume, which specifies the rotation matrix and the
translation vector. The world volume does not have a mother volume, and its coordinate
system is global.

A material in Geant4 is defined by successively defining the isotopes and elements. Iso-
topes are first defined to constitute an element with respective isotope abundances, e.g.,
enriched uranium. Different elements are used to define a material with corresponding ele-
ment fractions. For convenience, common materials are predefined in the internal material
database, which is derived from the National Institute of Standards and Technology (NIST).
This database consists of sub-libraries for single-element materials with natural isotope abun-
dance, NIST compounds, high energy physics and nuclear materials, space materials, and
bio-chemical materials, respectively.

3.4.2 Reference Physics List

The physics list class describes the particles and the physical processes associated with each
particle to be simulated in the calculation. Validated reference physics lists [55] for different
applications are provided, and recommendations for which lists to use for which applications
are provided. As an example, for neutrons under 20 MeV, the high-precision (HP) lists are
recommended, e.g., the **QGSP BERT HP** reference physics list.

The reference physics lists exclude optical physics, which may be needed to simulate
scintillation detectors. For this work, a modified physics list is used based on examples with
optical physics included with Geant4 source code, which demonstrates how to append the
optical physics to the selected reference physics list.
3.4.3 Action Initialization

In the action initialization class, the mandatory primary generator class and the optional user action classes are initialized. In the primary generator class, a concrete class derived from the base G4VPrimaryGenerator class is initialized to define source particles. Two concrete generator classes are provided, the G4ParticleGun and the G4GeneralParticleSource (GPS). The GPS class has all the functionality of G4ParticleGun and is more advanced. The GPS class defines a complete list of macro commands to define a variety of source particles. These generator classes can emit multiple source particles in a source event. Each source particle can have its own characteristic. As a comparison, in MCNP, a history typically consists of one source particle.

Objects of the optional user run, event, and step action classes can be linked to accumulate tallies. At the end of a step, the inherited UserSteppingAction function defined in the G4UserSteppingAction class is called to give access to basically all the information during this step, e.g., the total deposited energy along the step and coordinates of the start and the end step points. The information from all steps in a source event can be summed to a variable defined in the user event action to compute the event-specific tally. The event-specific tally can be further accumulated to the variables defined in the user run action to compute average and variance.

To illustrate the code structure of a Geant4 application and its similarities to (or differences from) typical MCNP models, both Geant4 and MCNP were used to model a simple source-detector system. The source code and inputs are provided in Appendix A.

3.5 Geant4 Optical Physics

The optical physics are constructed in the G4OpticalPhysics class, which is used to build the modified physics list as stated in Section 3.4.2. This class consists of seven optical processes that apply to the optical photon type, which is an independent particle type separate from the higher energy gamma photons that is used to simulate the wave-like electromagnetic
radiation. The seven optical processes are Cherenkov\textsuperscript{3}, scintillation, wave length shifting, optical absorption, Rayleigh scattering, Mie scattering, and optical boundary process. The first three are optical generation processes, and the last four are optical tracking processes. The Cherenkov and scintillation processes are implemented in the electromagnetic/xrays category, and the other five processes belong to the optical category in the Geant4 source tree. To simulate the scintillation detectors in this work, the optical absorption, the optical boundary, the scintillation, and the Cherenkov processes are of interest.

Polarization of optical photon must be specified for correct simulation of optical physics. The polarizations of the secondary optical photons are sampled by the kernel, i.e., from either the Cherenkov or the scintillation processes. If the optical photons are the source particles, the polarizations need to be specified by the user.

While algorithms for optical-photon transport are implemented, optical properties need to be supplied by the user. The optical physics are simulated only if optical processes are included in the physics list and the associated optical properties are provided. An optical property can be specified as a constant or as a function of energy. The majority of the non-constant optical properties depend on the optical photon energy, and the particle-dependent scintillation yields also depend on the deposited energy. An example in Geant4 is the variable that defines the light yield for protons named PROTONSCINTILLATIONYIELD. In the classes that implement optical processes, the \texttt{GetConstProperty} function is called to find the associated constant optical properties, and the \texttt{GetProperty} function is invoked to locate the needed energy-dependent optical properties. The associated optical properties with each optical process are summarized in Table 3.1.

### 3.5.1 Optical Absorption Process

The optical absorption process is implemented in the \texttt{G4OpAbsorption} class. It simulates the bulk absorption (compared to the surface absorption detailed later) when an optical photon travels in a material. This process reads the energy-dependent optical absorption length.

\textsuperscript{3}The spelling of \textit{Cerenkov} is used in Geant4 source code. However, the writing guidelines published by CERN [56] suggest the spelling \textit{Cherenkov}, which is adopted here.
Table 3.1: Summary of the optical properties read by each optical process. Properties with superscript \textsuperscript{c} are constants, and others are functions of optical photo or deposited energy. Data are extracted from the Geant4 source code.

<table>
<thead>
<tr>
<th>Optical process</th>
<th>Optical property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>absorption</td>
<td>\texttt{ABSLENGTH}</td>
<td>mean free path of optical absorption</td>
</tr>
<tr>
<td>boundary process</td>
<td>\texttt{RINDEX}</td>
<td>material refractive index</td>
</tr>
<tr>
<td></td>
<td>\texttt{INDEX}</td>
<td>surface refractive index (RI) of back-painted finishes \textsuperscript{[57]}</td>
</tr>
<tr>
<td></td>
<td>\texttt{REFLECTIVITY}</td>
<td>probability for an optical photon to be reflected or refracted at a surface</td>
</tr>
<tr>
<td></td>
<td>\texttt{REALRINDEX}</td>
<td>real part of RI to compute reactivity of a dielectric-metal surface</td>
</tr>
<tr>
<td></td>
<td>\texttt{IMAGINARYRINDEX}</td>
<td>imaginary part of RI to compute reactivity of a dielectric-metal surface</td>
</tr>
<tr>
<td></td>
<td>\texttt{EFFICIENCY}</td>
<td>probability of detecting an optical photon at a surface</td>
</tr>
<tr>
<td></td>
<td>\texttt{TRANSMITTANCE}</td>
<td>refraction probability (optional)</td>
</tr>
<tr>
<td></td>
<td>\texttt{SPECULARLOBECONSTANT}</td>
<td>probability of specular lobe reflection in a surface reflection event</td>
</tr>
<tr>
<td></td>
<td>\texttt{SPECULARSPIKECONSTANT}</td>
<td>probability of specular spike reflection in a surface reflection event</td>
</tr>
<tr>
<td></td>
<td>\texttt{BACKSCATTERCONSTANT}</td>
<td>probability of backscatter reflection in a surface reflection event</td>
</tr>
<tr>
<td></td>
<td>\texttt{GROUPvel}</td>
<td>final velocity of a refracted optical photon</td>
</tr>
<tr>
<td></td>
<td>\texttt{SURFACEROUGHNESS} \textsuperscript{c}</td>
<td>used to sample the probability of Lambertian reflection</td>
</tr>
<tr>
<td>Cherenkov</td>
<td>\texttt{INDEX}</td>
<td>refractive index</td>
</tr>
<tr>
<td>scintillation</td>
<td>\texttt{FASTCOMPONENT}</td>
<td>scintillator emission spectrum of the fast component</td>
</tr>
<tr>
<td></td>
<td>\texttt{SLOWCOMPONENT}</td>
<td>scintillator emission spectrum of the slow component</td>
</tr>
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<td>\texttt{PROTONSCINTILLATIONYIELD}</td>
<td>scintillation yield by proton</td>
</tr>
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<td>\texttt{DEUTERONSCLINTILLATIONYIELD}</td>
<td>scintillation yield by deuteron</td>
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<td>scintillation yield by triton</td>
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<td>scintillation yield by alpha</td>
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<td>scintillation yield by ion</td>
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<td>scintillation yield by electron</td>
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<td></td>
<td>\texttt{SCINTILLATIONYIELD} \textsuperscript{c}</td>
<td>number of optical photons per unit deposited energy</td>
</tr>
<tr>
<td></td>
<td>\texttt{RESOLUTIONSCALE} \textsuperscript{c}</td>
<td>scaler characterizing fluctuation of emitted optical photon number</td>
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<td>\texttt{FASTTIMECONSTANT} \textsuperscript{c}</td>
<td>decay time constant of fast component</td>
</tr>
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<td></td>
<td>\texttt{FASTSCINTILLATIONRISETIME} \textsuperscript{c}</td>
<td>rise time of fast component</td>
</tr>
<tr>
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<td>\texttt{SLOWTIMECONSTANT} \textsuperscript{c}</td>
<td>decay time constant of slow component</td>
</tr>
<tr>
<td></td>
<td>\texttt{SLOWSCINTILLATIONRISETIME} \textsuperscript{c}</td>
<td>rise time of slow component</td>
</tr>
<tr>
<td></td>
<td>\texttt{YIELDRATIO} \textsuperscript{c}</td>
<td>relative strength of fast component</td>
</tr>
<tr>
<td>Rayleigh scattering</td>
<td>\texttt{RAYLEIGH}</td>
<td>mean free path before Rayleigh scattering</td>
</tr>
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<td>\texttt{INDEX}</td>
<td>reflective index (RI)</td>
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<td>\texttt{ISOTHERMAL_COMPRESSIBILITY} \textsuperscript{c}</td>
<td>compressibility</td>
</tr>
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<td>\texttt{RS_SCALE_FACTOR} \textsuperscript{c}</td>
<td>optional scaler for the Rayleigh scattering length</td>
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<td>Mie scattering</td>
<td>\texttt{MIEHG}</td>
<td>mean free path of Mie scattering</td>
</tr>
<tr>
<td></td>
<td>\texttt{MIEHG_FORWARD} \textsuperscript{c}</td>
<td>average cosine of the forward angle</td>
</tr>
<tr>
<td></td>
<td>\texttt{MIEHG_BACKWARD} \textsuperscript{c}</td>
<td>average cosine of the backward angle</td>
</tr>
<tr>
<td></td>
<td>\texttt{MIEHG_FORWARD_RATIO} \textsuperscript{c}</td>
<td>ratio factor between the forward angle and backward angle</td>
</tr>
<tr>
<td>WLS</td>
<td>\texttt{WLSCOMPONENT}</td>
<td>relative emission spectrum</td>
</tr>
<tr>
<td></td>
<td>\texttt{WLSABSLENGTH}</td>
<td>absorption length</td>
</tr>
<tr>
<td></td>
<td>\texttt{WLSMEANNUMBERPHOTONS} \textsuperscript{c}</td>
<td>mean number of secondary OPs following Poisson distribution</td>
</tr>
<tr>
<td></td>
<td>\texttt{WLSTIMECONSTANT} \textsuperscript{c}</td>
<td>time delay between absorption and re-emission</td>
</tr>
</tbody>
</table>

\texttt{(ABSLENGTH)}, which defines the mean free path of an optical photon in a specific material.

This process is needed, for example, to simulate optical transport through ZnS(Ag), which absorbs its scintillation light.
3.5.2 Optical Boundary Process

The optical boundary process is implemented in the \texttt{G4OpBoundaryProcess} class. This process simulates the behavior of an optical photon at the boundary between two different materials. An optical photon can be absorbed, reflected, or refracted, sampling of which depends on the optical surface property. An optical surface is defined by its model, finish, type, and the parameter $\sigma_\alpha$, which defines surface roughness. A model is the algorithm to sample the optical boundary process, and the \texttt{glisur}, \texttt{unified}, \texttt{LUT} (look-up-table) and \texttt{dichroic} models are provided. The unified model is used in the DETECT program [58], and it applies to the dielectric-dielectric surface. This model was adopted for all simulations performed as part of the present work.

The available surface finishes are listed in Table 3.2. For this work, the polished, polishedfrontpainted, and ground finishes were used. For a ground surface, $\sigma_\alpha$ is used to sample the polar angle $\vartheta$ between a virtual facet and the physical average surface, i.e., $\vartheta$ follows a normal distribution, the mean and standard deviation of which are zero and $\sigma_\alpha$, respectively. The azimuthal angle $\psi$ is uniformly sampled from zero to $2\pi$. Then, the solid angle $\Omega$ are computed as

$$\Omega = i \sin \vartheta \cos \psi + j \sin \vartheta \sin \psi + k \cos \vartheta.$$  \hspace{1cm} (3.10)

The solid angle and the normal of the average physical surface are used to calculate the normal of the facet, and the boundary processes are with respect to the sampled facet. The virtual facet is not defined, and only its normal vector is sampled on-the-fly. As a comparison, the physical average surface exists in the tracking geometry, i.e., the surrounding surface of a volume defined in the detector construction class.

The supported surface types are dielectric-metal, dielectric-dielectric, dielectric-LUT (dielectric-Look-Up-Table interface), dielectric-dichroic (dichroic filter interface), firsov (for Firsov process), and xray (for x-ray mirror process). The dielectric-dielectric type was used for this work because the PMMA and ZnS(Ag) are dielectric materials.
Table 3.2: Optical surface finishes in Geant4. Data are extracted from the Geant4 source code.

<table>
<thead>
<tr>
<th>Finish</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>polished</td>
<td>smooth perfectly polished surface</td>
</tr>
<tr>
<td>polishedfrontpainted</td>
<td>smooth top-layer (front) paint</td>
</tr>
<tr>
<td>polishedbackpainted</td>
<td>same as 'polished' but with a back-paint</td>
</tr>
<tr>
<td>ground</td>
<td>rough surface</td>
</tr>
<tr>
<td>groundfrontpainted</td>
<td>rough top-layer (front) paint</td>
</tr>
<tr>
<td>groundbackpainted</td>
<td>same as 'ground' but with a back-paint</td>
</tr>
<tr>
<td>polishedlumirrorair</td>
<td>mechanically polished surface, with lumirror</td>
</tr>
<tr>
<td>polishedlumirrorglue</td>
<td>mechanically polished surface, with lumirror and meltmount</td>
</tr>
<tr>
<td>polishedair</td>
<td>mechanically polished surface</td>
</tr>
<tr>
<td>polishedteflonair</td>
<td>mechanically polished surface, with teflon</td>
</tr>
<tr>
<td>polishedtioair</td>
<td>mechanically polished surface, with tio paint</td>
</tr>
<tr>
<td>polishedtyvekair</td>
<td>mechanically polished surface, with tyvek</td>
</tr>
<tr>
<td>polishedvm2000air</td>
<td>mechanically polished surface, with esr film</td>
</tr>
<tr>
<td>polishedvm2000glue</td>
<td>mechanically polished surface, with esr film and meltmount</td>
</tr>
<tr>
<td>etchedlumirrorair</td>
<td>chemically etched surface, with lumirror</td>
</tr>
<tr>
<td>etchedlumirrorglue</td>
<td>chemically etched surface, with lumirror and meltmount</td>
</tr>
<tr>
<td>etchedair</td>
<td>chemically etched surface</td>
</tr>
<tr>
<td>etchedteflonair</td>
<td>chemically etched surface, with teflon</td>
</tr>
<tr>
<td>etchedtioair</td>
<td>chemically etched surface, with tio paint</td>
</tr>
<tr>
<td>etchedtyvekair</td>
<td>chemically etched surface, with tyvek</td>
</tr>
<tr>
<td>etchedvm2000air</td>
<td>chemically etched surface, with esr film</td>
</tr>
<tr>
<td>etchedvm2000glue</td>
<td>chemically etched surface, with esr film and meltmount</td>
</tr>
<tr>
<td>groundlumirrorair</td>
<td>rough-cut surface, with lumirror</td>
</tr>
<tr>
<td>groundlumirrorglue</td>
<td>rough-cut surface, with lumirror and meltmount</td>
</tr>
<tr>
<td>groundair</td>
<td>rough-cut surface</td>
</tr>
<tr>
<td>groundteflonair</td>
<td>rough-cut surface, with teflon</td>
</tr>
<tr>
<td>groundtioair</td>
<td>rough-cut surface, with tio paint</td>
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<tr>
<td>groundtyvekair</td>
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</tr>
<tr>
<td>groundvm2000air</td>
<td>rough-cut surface, with esr film</td>
</tr>
<tr>
<td>groundvm2000glue</td>
<td>rough-cut surface, with esr film and meltmount</td>
</tr>
</tbody>
</table>

When an optical surface is defined, it can be assigned to the physical surface of a defined volume as a skin surface or a border surface. The optical properties of a skin surface are used to simulate the optical boundary processes for photons coming from both sides of the physical surface. The border surface is one-way transport. Two border surfaces can be used to describe different optical properties of the two faces of one physical surface, respectively. For example, two border surfaces can be used to simulate a box with an inner surface painted...
black and an outer surface painted white. The optical photons coming from outside the box are reflected, and the ones coming from inside the box are absorbed.

An optical photon can be reflected, refracted (transmitted), or absorbed at the boundary. The probability that an optical photon is not absorbed at the surface is defined via the \textbf{reflectivity} parameter of the optical surface. If an optical photon is not absorbed, it is reflected at a painted surface. At other surfaces, the optical photon that survives is reflected or refracted.

Reflection and refraction at a polished surface are illustrated in Fig. 3.2. The reflection angle $\theta_r$ equals the incident angle $\theta_i$. The refracted angle $\theta_t$ is calculated by the Snell’s law, i.e.,

$$n_1 \sin \theta_i = n_2 \sin \theta_t,$$

where $n_1$ and $n_2$ are the refractive indices of the two materials. The reflection probability $R$ for an optical photon with incident angle $\theta_i$ is [58]

$$R = \frac{1}{2} \left[ \frac{\sin^2(\theta_i - \theta_t)}{\sin^2(\theta_i + \theta_t)} + \frac{\tan^2(\theta_i - \theta_t)}{\tan^2(\theta_i + \theta_t)} \right],$$

and the refraction probability $T$ is

$$T = 1 - R.$$

The reflection and refraction probabilities also apply to a ground surface except that the angles are defined with respect to the sampled micro facet.

If an optical photon is sampled to be reflected at a ground surface using the unified model, the reflection type is further sampled to be specular spike, specular lobe, backscatter, or Lambertian [57, 59]. The specular spike reflection is with respect to the physical average of the ground surface, as shown in Fig. 3.2. The specular lobe reflection is similar to specular spike except that it is with respect to the sampled facet. These two specular reflections are implemented together in the \texttt{G4OpBoundaryProcess} class using respective surface normal vectors. In the backscatter reflection, the optical photon is reflected back to the incident direction. In the Lambertian reflection, the optical photon can be reflected into any direction.
Figure 3.2: An optical photon is reflected or refracted at a polished boundary.

in the surface hemisphere, as shown in Fig. 3.3.

Probabilities of the specular spike, specular lobe, and backscatter reflections are defined via the SPECULARSPIKECONSTANT, SPECULARLOBECONSTANT, and BACKSCATTERCONSTANT inputs, respectively. The Lambertian reflection is implicit, i.e., its probability equals to one minus the sum of the three constants. This setting ensures the sum of the four reflection probabilities is unity to preserve the relative probabilities of reflection or refraction, as shown in Eq. (3.12) and Eq. (3.13). If the three constants are not specified, the Lambertian reflection is assumed.
3.5.3 Scintillation Process

The scintillation process is implemented in the \texttt{G4Scintillation} class. The average number of emitted optical photons per deposited energy can be defined via the \texttt{SCINTILLATIONYIELD} constant. The scintillation yield can also be defined to be dependent on particle type and deposited energy. For example, the scintillation yield for protons can be defined via \texttt{PROTONSCINTILLATIONYIELD} as a function of deposited energy. The other supported particles are deuteron, electrons, deuterons, tritons, alphas, and carbon ions [60]. The associated inputs are shown in Table 3.1. The scintillation yield ($SY$) is used to compute the mean number of scintillation photons $N_m$, i.e.,

$$N_m = dE \cdot SY,$$  

where $dE$ is the deposited energy. For $N_m$ larger than 10, the actual number of emitted photons $N$ in a Monte Carlo step follows a Gaussian distribution with a standard deviation $\sigma_g$ calculated from \texttt{RESOLUTIONSCALE}, i.e.,

$$\sigma_g = \texttt{RESOLUTIONSCALE} \cdot \sqrt{N_m}.$$  

For $N_m \leq 10$, $N$ is sampled from Poisson distribution.

The scintillation photons may have fast and slow components. The emission spectrum of the fast component is specified by the \texttt{FASTCOMPONENT} array as a function of optical photon energy. The decay time constant and the rise time of the fast component are specified via \texttt{FASTTIMECONSTANT} and \texttt{FASTSCINTILLATIONRISETIME}, respectively. These properties of the slow component can be specified via corresponding inputs. The probability of a scintillation photon born into the fast component is specified by the \texttt{YIELDRATIO} parameter.
3.6 Summary

In this chapter, fundamentals of the Monte Carlo simulation were presented. The Monte Carlo method is endorsed by the law of large numbers and the central limit theorem. In a Monte Carlo simulation of particle transport, a general flow consists of sampling the free path, reaction nuclide at the collision site, and reaction type based on respective cross sections.

To model and simulate the neutron detectors in this work, the Geant4 Monte Carlo code is used. The code structure of the detector models was described. In addition, the Geant4 optical physics used to simulate the scintillation detectors were reviewed. The user-supplied optical properties read by each optical process were summarized. In particular, the optical absorption, boundary, and scintillation processes were discussed. In the following chapters, Geant4 and other codes will be used to model and simulate neutron detectors developed for TREAT.
Chapter 4

Hornyak Button Neutron Detector

The “Hornyak button” is a simple, fast neutron detector constructed from a mixture of ZnS and Lucite first proposed by Hornyak in 1951 [61]. Variants of these detectors [11] were used in the original TREAT hodoscope and are again in use (after refurbishment) at TREAT following the restart of reactor operations. In this chapter, a model constructed using Geant4 is described that was used to simulate the performance of the Hornyak buttons in assumed, hodoscope-like conditions, in which the coupled nuclear and optical physics in the detector were accounted for explicitly. The computed results are compared with reported experimental data to provide a preliminary validation of the computational methodology and physics models used.

4.1 Description of the Hornyak Button

Shown in Fig. 4.1 is the geometry of the Hornyak button detectors used in the original TREAT hodoscope [11]. The devices consist of a scintillation volume sandwiched between two polymethyl methacrylate (PMMA) light guides. The scintillation volume contains a uniform mixture of ZnS(Ag) (5% by mass) and PMMA, whose chemical formula and density are \((C_5O_2H_8)_n\) and 1.19 g/cm\(^3\), respectively. A PMT is connected to the end of the device (not shown in Fig. 4.1) to collect and amplify the scintillation light. The surfaces not
connected to the PMT are painted white to maximize light retention within the light guide.

Figure 4.1: Schematic of the Hornyak button as used at TREAT (after [Ref. 11]).

A fast neutron entering the scintillation volume has a certain probability to interact with the hydrogen in the PMMA and to generate a recoil proton via elastic scattering. If a ZnS(Ag) grain exists along the path of the recoil proton, energy is deposited in the scintillator, and light is emitted. The light may leave the scintillation volume, be reflected at the white, outer surfaces of the light guide, and reenter the scintillation volume several times before arriving at the PMT. In the scintillation volume, the light may be absorbed by ZnS(Ag). If a sufficient amount of light reaches the PMT to generate a pulse with height larger than the LLD setting, the neutron is detected. The polished, cylindrical light guides yield reasonably good light-collection efficiency along the 1-inch length of the scintillation volume. For neutrons above 0.1 MeV, the Hornyak buttons used at TREAT were observed to have an efficiency of approximately 0.4% [11].

The Hornyak buttons were reported to suffer from large gamma-induced Cherenkov noise generated in the light guides and the photomultiplier glass envelope [11]. The gamma rays may interact within the Hornyak button to generate electrons via the photoelectric effect,
Compton scattering, and pair production. These electrons can subsequently generate scintillation and Cherenkov noise light. Considering the relatively long range of the electrons, only a small fraction of the gamma energy is expected to be transferred to the ZnS(Ag). Therefore, the scintillation noise is relatively easy to eliminate by pulse-height discrimination. However, because the light guides and the photomultiplier glass envelope consist of a large volume fraction of the device, production of Cherenkov light is high. The overwhelming Cherenkov noise may have contributed to the nonlinearity between the detector response and the TREAT neutron monitors during large transient experiments [11]. To reject the Cherenkov noise, a pulse-shaping technique was developed based on the decay time difference between the scintillation light and the Cherenkov light [29]. Additionally, lead filters were used in front of the detectors to attenuate the gamma rays and to help eliminate the nonlinearity [11]. These techniques, though successful, complicated the detection system.

4.2 Hodoscope Radiation Environment

To simulate the performance of Hornyak button, the radiation environment in the hodoscope must be approximated using available information. As stated in Section 1.2.7, the hodoscope detectors are designed to measure mono-directional, fast neutrons coming through the channels and to suppress the gamma rays generated from the neutron capture reaction in the steel collimator. While prompt fission gamma rays were present with an intensity of approximately 5 per fission neutron, these gamma rays may contribute to the prompt signal used to identify fuel motion. However, for the work described here, the rejection of all gamma rays was maximized. In addition to the prompt, fission gamma rays, the intensity of the neutron-activation gamma rays was about 9 additional gamma rays per fission neutron [11]. These gamma rays originated from neutron activation were modeled as the background radiation in the calculations.

Because it would be nearly impossible to simulate the original TREAT hodoscope environment, it was decided to define a representative neutron and gamma-ray radiation field that is believed to be conservative. Specifically, neutrons were assumed to be mono-directional
and perpendicular to a detector’s front face (i.e., the face adjacent to a collimator channel).

Neutron energies were assumed to follow a $^{235}\text{U}$ thermal, Watt fission spectrum [62], i.e., for neutron energy $E$ in MeV, the probability $f$ is

$$f(E) \propto \exp(-E/0.988) \sinh(\sqrt{2.249E}).$$ \hspace{1cm} (4.1)

This spectrum is shown in Fig. 4.2.

For each source neutron incident on the detector, it was assumed that 10 gamma rays were simultaneously incident on the detector. For different detector form factors in this work, this neutron-to-gamma ratio was maintained by adapting the number of gamma rays in a pulse event. The gamma rays were assumed to be isotropically distributed in angle and to follow a fission gamma-ray spectrum in energy, i.e., the probability $G$ of gamma rays with
energy $E$ in MeV follows \[63\]

$$G(E) = \begin{cases} 
38.13(E - 0.085)e^{1.648E} & E < 0.3 \\
26.8e^{-2.3E} & 0.3 < E < 1.0 \\
8.0e^{-1.1E} & 1.0 < E < 8.0 
\end{cases}, \quad (4.2)$$

which is shown in Fig. 4.2. Finally, the neutron and gamma-ray sources were assumed to be distributed uniformly in space over the detector’s entire front face.

### 4.3 Hornyak Button Model

#### 4.3.1 ZnS(Ag) Grain Randomization

The Hornyak button model developed using Geant4 is shown in Fig. 4.3. The light guides were modeled as two sectors, each with a central angle of 160° [11]. To model the homogeneous mixture of ZnS(Ag) and PMMA in the scintillation volume, ZnS(Ag) grains were modeled as spheres with a radius of 20 µm [64]. Only the reported average radius was used because information for grain size distribution is not known from the literature. Indeed, the effects of the grain size on detector performance may need to be evaluated (but were not considered in this work). Based on a 5% mass fraction of ZnS(Ag) [11], the number of ZnS(Ag) grains $N_g$ in the scintillation volume was computed to be about $5 \times 10^5$.

To randomly distribute the $N_g$ grains into the scintillation volume efficiently, a pseudo-randomization method was used. The scintillation volume was divided into $N_x$, $N_y$, and $N_z$ layers along the $x$, $y$, and $z$ axes, respectively. The alignment of the scintillation volume with respect to the axes is shown in Fig. 4.1. The number of layers along an axis was proportional to the corresponding dimension of the scintillation volume, i.e.,

$$\frac{N_x}{L_x} = \frac{N_y}{L_y} = \frac{N_z}{L_z}, \quad (4.3)$$

where $L_x = 5/8$, $L_y = 7/64$, and $L_z = 1$ inch (see Fig. 4.1). These layers formed $N_x \times N_y \times$
\[ N_z = N_g \text{ cells, and a cell contained one ZnS(Ag) grain.} \]

As computed, the numbers of layers are not integers, while the number of grains along an axis must be an integer. Hence, the scintillation volume was first divided into \( \tilde{N}_z \) layers along the \( z \) axis, where \( \tilde{N}_z \) was the integer part of \( N_z \). Then, each \( z \) layer contained \( N_{xy} = N_g / \tilde{N}_z \) grains. The values of \( N_x \) and \( N_y \) were recomputed by

\[
N_{xy} = N_x \times N_y \\
N_x / L_x = N_y / L_y.
\]

Then, the number of \( y \) layers in a \( z \) layer was sampled to be \( \tilde{N}_y + 1 \) with probability \( N_y - \tilde{N}_y \) or \( \tilde{N}_y \) otherwise, where \( \tilde{N}_y \) is the integer part of \( N_y \). The number of \( x \) layers was sampled in the same way. A ZnS(Ag) grain was randomly embedded in each cell if it did not overlap with the neighbor placed grains. If placement of a grain in a cell failed 100 times, i.e., all the sampled positions of the grain overlapped with the neighbor grains, that cell was left as void, and the number of placed grains was counted. The volume of the scintillation volume not occupied by the ZnS(Ag) grains (including the void cells) was filled with PMMA. This pseudo-randomization method avoided issues with overlapping ZnS(Ag) grains and ensured that desired mass fractions were preserved to within approximately 0.2% of the desired value for the cases studied. Figure 4.3b shows the random distribution of the ZnS(Ag) grains of the model.

A dummy, finite-volume PMT was connected to the end window of the Hornyak button (not shown in Fig. 4.3a). If an optical photon left the Hornyak button and entered the PMT region, the particle was killed, and the tally, i.e., number of detected optical photons in an event, was increased by one.

### 4.3.2 Optical Surface Settings

The outer surface of a ZnS(Ag) grain was modeled as ground, and the polished-front-painted surface finish in Geant4 [59] was used to model the optical reflective property of the outer
surfaces of the light guides [11]. All other surfaces, e.g., the surfaces between the scintillation volume and the light guides and the surface between the Hornyak button and the PMT, were modeled as polished [11, 57]. Because all the surfaces except the coupling ones in the Hornyak button were coated with white reflective paint [11], no surface absorption of optical photons was considered. All surfaces were assumed to be of the dielectric-dielectric type.

4.3.3 Source Planes

To simulate neutron responses, prompt neutrons were born uniformly in the cross-sectional plane of the scintillation volume (Fig. 4.4a). For gamma-induced scintillation, 10 gamma rays per source neutrons were also sampled uniformly across the cross-sectional plane of the scintillation volume. However, because Cherenkov radiation is generated in both the scintillation region and the light guides, incident gamma rays were sampled across the entire
cross-sectional area of the Hornyak button (Fig. 4.4b) in order to simulate the response due to Cherenkov radiation. To maintain a consistent gamma-ray intensity between the two cases, the number of gamma rays per event for the Cherenkov study was

\[
N = \frac{\text{Cross-sectional area of the detector}}{\text{Cross-sectional area of the scintillation volume}} \times 10 \approx 69. \quad (4.5)
\]

Figure 4.4: One neutron per event was generated uniformly in source plane 1. To evaluate the gamma-induced scintillation noise, 10 gamma rays per event were generated uniformly in source plane 1. To evaluate the gamma-induced Cherenkov noise and the combined Cherenkov-scintillation noise, 69 gamma rays per event were born uniformly in source plane 2.

4.4 Physical Models and Approximations

Geant4 version 10.2 with patch 02 [32] was used to simulate the Hornyak button and other ZnS(Ag)-based detectors presented in the next chapter. Neutron interactions were based on the neutron cross-section file G4NDL4.5. Nuclear processes were simulated using the recommended QGSP BERT HP physics list [55], and all necessary optical processes, e.g., optical absorption, scintillation, Cherenkov, and boundary interactions (using the UNIFIED model), were taken into account. For gamma-ray calculations, scintillation and Cherenkov processes were enabled independently so that scintillation noise, Cherenkov noise, and their combination were analyzed separately.

The refractive index of PMMA is a known function of wavelength [65], with an average value of approximately 1.49. For ZnS(Ag), the refractive index was set to 2.36, while the
mean free path of the optical photons in ZnS(Ag) was set to 13 µm [66]. The light yield of ZnS(Ag) was set to 37 optical photons per keV [67] with an emission spectrum maximized at a 450-nm wavelength [68]. For all cases, millions of source-particle events were simulated to obtain good statistics.

4.5 Tally Method

The pulse heights of the Hornyak button and the variants discussed in the next chapter were represented by the number of detected optical photons (OPs). An optical photon that travels to the photon-detection device was recognized as detected because of the high PMT and SiPM (for Hornyak variants evaluated in the next chapter) photon-detection efficiency [9] for optical photons following the ZnS(Ag) emission spectrum [68]. Pulse height distributions of these ZnS(Ag)-based scintillation detectors were formed using the Analysis class in Geant4 with comma-separated values (CSV) output format. The generated CSV files were post processed using Python scripts.

4.6 Detector Response and Efficiency

The pulse height distributions of neutron and gamma events were simulated in different runs. The signal pulse height distribution by neutrons was computed in a run. The pulse height distribution by gamma rays considering scintillation, Cherenkov, and the combination of these two processes were calculated in three runs, respectively. The source information in these runs is specified in Section 4.3.3.

Based on the signal and noise pulse height distributions, an appropriate LLD can be set to reject a majority of the gamma noise. In the scintillation detectors, the LLD setting was represented by the number of detected optical photons. At the selected LLD setting, the neutron-detection efficiency can be calculated, which quantified the detector performance.
Specifically, the detection efficiency $\varepsilon$ at an LLD setting was computed as

$$\varepsilon = \frac{\text{Number of pulses with height larger than LLD}}{\text{Total number of pulses}}.$$

(4.6)

Corresponding to different LLD settings, the coupled neutron-detection efficiency $\varepsilon_n$ and gamma-detection efficiency $\varepsilon_g$ can be computed, with an associated signal-to-noise (S/N) ratio defined as

$$\text{S/N ratio} = \frac{\varepsilon_n}{\varepsilon_g}.$$

(4.7)

To evaluate the hodoscope detectors, if not specified explicitly, the neutron-detection efficiency was defined using an LLD setting consistent with an S/N ratio of 100. It is understood an S/N ratio of 100 with respect to the background gamma rays is a desirable functional capability of advanced fast-neutron detectors for the hodoscope [69], and, hence, it is believed that the neutron-detection efficiency defined in this way is a practical value.

### 4.7 Results

Shown in Fig. 4.5 are the predicted pulse-height spectra and neutron-detection efficiencies for the Hornyak button. As indicated by Fig. 4.5a, the neutron event pulse height distribution is flatter than that of the scintillation noise, which makes pulse-height discrimination of the scintillation noise possible at reasonably low LLD settings. Contrarily, the intense Cherenkov noise is readily apparent and dominates the gamma-ray background. Figure 4.5b shows that for a wide range of LLD settings, the neutron-detection efficiency is on the order of 0.1%. One factor causing the relatively low neutron-detection efficiency is the small amount of energy deposited in the scintillator. According to the calculation, on average, each neutron resulted in approximately 5-keV energy deposited in the ZnS(Ag). This limited energy deposition may be due to the relative low concentration of the ZnS(Ag) in the scintillation volume, which results from the compromise between light generation and light absorption.

Furthermore, if it is assumed the Cherenkov noise is rejected by the pulse-shaping tech-
nique, as discussed in Section 1.2.8, an LLD setting of 180 optical photons can achieve an S/N ratio of 100 with respect to gamma-induced scintillation noise, and the corresponding neutron-detection efficiency is about 0.35%, as shown in Fig. 4.5b. It was reported that the neutron-detection efficiency of Hornyak button was approximately 0.1%, or, for neutrons above 0.1 MeV, the value is approximately 0.4% with pulse-shape discrimination to reject the gamma-induced Cherenkov noise [11]. Hence, the simulated results are in relatively good agreement with the reported values, an agreement that provides some validation of the methodology used.

If both gamma-induced scintillation and Cherenkov contributions are included, to achieve an S/N ratio of 100, an LLD setting of 645 optical photons is necessary, and the corresponding neutron-detection efficiency is about 0.086%, as shown in Fig. 4.5b. In realistic application, the Cherenkov noise may even be stronger because it can also be generated in the glass envelope of the PMT [11] but was not considered in the calculation. Hence, the results verify the necessity of the pulse-shaping technique to reject the Cherenkov noise, which may contribute to the non-linear detector response with increased reactor power during transient experiments [11].

4.8 Summary

In this chapter, the traditional Hornyak button fast-neutron detector used in the hodoscope was evaluated in Geant4, where the coupled nuclear and optical transports were simulated. For assumed, hodoscope-like conditions, an intrinsic efficiency of 0.35% for mono-directional fission neutrons was predicted. The predicted efficiency is in reasonably good agreement with experimental data from the literature. Strong Cherenkov noise was also observed in the simulation. If the LLD was set to reject the gamma-induced scintillation and Cherenkov noises generated in the Hornyak button, the neutron-detector efficiency reduces to about 0.086%. The Cherenkov noise is even stronger if the contribution from PMT was considered. These results validate the physics models and approximations employed, and the simulation techniques will be used to evaluate the proposed Hornyak variants in the next chapter.
Figure 4.5: Results of the original Hornyak button model.
Chapter 5

Hornyak Button Variants

Although the Hornyak button used at TREAT is simple in design and function, the signal ultimately acquired would be improved by designs exhibiting a higher neutron-detection efficiency and/or a higher signal-to-noise ratio (e.g., through the production of less Cherenkov radiation). Here, two variants of the Hornyak button are proposed and studied. The first is an extension of the existing Hornyak button based on an optimal, homogenized mixture of ZnS(Ag) and Lucite. The second uses alternating layers of ZnS(Ag) and Lucite of optimal thicknesses to maximize light transport in the directions orthogonal to the beam line. The new detectors use SiPMs to collect light, which is more efficient than the combination of light guides and the PMT used in the Hornyak button and reduces the Cherenkov noise. The improved light-collection method allows a higher concentration of ZnS(Ag) in the homogenized or the layered scintillation volumes to increase the neutron-detection efficiency. In this chapter, these new detectors are evaluated in Geant4 to demonstrate the designs.

5.1 Design of the Variants

Shown in Fig. 5.1 are the schematics of the layered and the homogenized detectors. SiPMs are used to replace the light guides and PMT used in Hornyak buttons, which reduces generation of the Cherenkov noise and overall detector mass and volume. Therefore, the gamma
background in the TREAT hodoscope may be rejected by use of pulse-height discrimination alone, and the more complicated, pulse-shaping techniques used with the Hornyak buttons may not be necessary.

The use of SiPMs simplifies the light collection process. In the Hornyak button, the majority of the scintillation light needs to be reflected at the cylindrical surfaces of the light guides and may re-enter the scintillation volume several times to reach the PMT placed at the far end of the device (see Fig. 4.1). Each time the light passes through the scintillation volume, it may be absorbed by the relatively opaque ZnS(Ag). By using SiPMs in the new detectors, the scintillation light that leaves the scintillation volume can be directly detected. Hence, the new light collection method is more efficient.

Figure 5.1: Geometric illustrations of the two new detectors. The cross-sectional area of both scintillation volumes is a rectangle with size $2.51 \times 8.89$ mm, which is consistent with the designed channel slit in the TREAT hodoscope.
The improved light collection method allows better scintillation volume design. For the homogenized detector, the scintillation volume is a Hornyak-button-like mixture of PMMA and ZnS(Ag). Because of the new light collection method, use of a higher concentration of ZnS(Ag) in the scintillation volume is possible, which increases overall light production and leads to better maximum performance.

For the layered detector, the scintillation volume consists of repeated layers of ZnS(Ag) and PMMA. The layered configuration is more efficient for the forward-directional, recoil protons to deposit energy in the ZnS(Ag) layers compared to the homogenized scintillation volume, where a proton may not encounter a randomly-distributed ZnS(Ag) grain along its path and, therefore, cannot generate a signal pulse.

While the homogenized scintillation volume is less efficient for the forward-directed protons to deposit energy in the scintillator than the layered configuration, this inefficiency may contribute to improved gamma-ray rejection. As the ratio of background gamma rays to incident neutrons increases, the corresponding S/N ratio decreases faster for the layered detector than for the homogenized detector. Hence, the homogenized detector will exhibit better performance in a highly intense gamma-ray background environment (beyond what is actually expected in the hodoscope environment).

In the following sections, the Hornyak variants were optimized and evaluated using techniques detailed in Chapter 4. In particular, the new detectors were irradiated by the neutron and gamma sources that represent the hodoscope radiation environment, as detailed in Section 4.2. Except the gamma rejection evaluations, in a pulse event, one neutron and 10 gamma photons were born uniformly in the detector’s cross-sectional plane (a $2.52 \times 8.89$ mm rectangle) to preserve the hodoscope radiation environment, and the renormalization of the number of gamma photons (as in the evaluation of the Hornyak button, Section 4.3.3) was not needed. The neutron-detection efficiencies were defined at LLD settings achieving S/N ratio of 100, where gamma-induced Cherenkov and scintillation noises were considered.
5.2 Layered Detector Results

5.2.1 Thickness Optimization

The primary variables affecting the layered detector performance are the thicknesses of the PMMA and the ZnS(Ag) layers. While a thick PMMA layer enhances the proton generation and light collection, a large percentage of the recoil protons cannot escape the layer and are wasted. According to SRIM [39], the projected range of a 2-MeV proton in PMMA is about 65 \( \mu \)m. Additionally, a thick ZnS(Ag) layer is beneficial for maximizing the energy deposited by entering protons but leads to increased self-absorption of light. Hence, a parametric study was performed to find the optimal thicknesses of the PMMA and ZnS(Ag) layers for a representative 5-cm long layered device. The ZnS(Ag) layers were modeled with ground optical surfaces, while the surfaces of the PMMA layers were modeled as polished.

Table 5.1 summarizes the PMMA and ZnS(Ag) layer thicknesses considered that can yield a neutron-detection efficiency above 2\%. The gamma-induced noises by the scintillation and Cherenkov processes were used to set the LLD. The best case, where the thicknesses of the PMMA layer and the ZnS(Ag) layer are 0.18 mm and 12 \( \mu \)m, respectively, can yield an efficiency of about 3.31\%.

Table 5.1: The neutron-detection efficiencies (\%) of a 5-cm long, layered detector under different layer thicknesses.

<table>
<thead>
<tr>
<th>PMMA (mm)</th>
<th>ZnS(Ag) (( \mu )m)</th>
<th>2</th>
<th>4</th>
<th>7</th>
<th>12</th>
<th>21</th>
<th>35</th>
<th>59</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td></td>
<td>2.05</td>
<td>3.02</td>
<td>3.15</td>
<td>2.49</td>
<td>2.21</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.18</td>
<td></td>
<td>2.44</td>
<td>3.03</td>
<td>3.26</td>
<td>3.31</td>
<td>2.71</td>
<td>2.06</td>
<td></td>
</tr>
<tr>
<td>0.32</td>
<td></td>
<td>2.16</td>
<td>2.47</td>
<td>2.54</td>
<td>2.61</td>
<td>2.43</td>
<td>2.11</td>
<td></td>
</tr>
</tbody>
</table>

5.2.2 Pulse Height Distributions

Figure 5.2 shows the pulse-height distribution and the neutron-detection efficiencies for a 5-cm long device with the optimum layer thicknesses. The gamma-induced noise is primarily introduced through scintillation, whereas the Cherenkov noise is minimal and easily rejected.
In other words, a pulse-shaping technique as used for the Hornyak button is not necessary. Moreover, over a wide range of LLD settings, the neutron-detection efficiencies are larger than 1% (Fig. 5.2b). At an LLD setting of 180 optical photons, the S/N is predicted to be 100, including both scintillation and Cherenkov, with a corresponding neutron-detection efficiency of approximately 3.31%.

Figure 5.2: Performance of the 5-cm long, optimized layered detector.
5.2.3 Length Evaluation

Better efficiency is expected by increasing the length of the layered detector, and a study was performed to determine the neutron-detection efficiency as a function of the detector length with the PMMA and ZnS(Ag) layer thicknesses set to the best-case values; the results are shown in Figure 5.3. LLDs that achieved an S/N ratio of 100 were set. At a length of one inch (the same length as the Hornyak buttons deployed at TREAT), the layered detector can yield a neutron-detection efficiency of approximately 1.8%. This improved performance (relative to the Hornyak button efficiency of 0.4%) may be explained by the increased energy deposition in the scintillator. At this length, the average energy deposited in ZnS(Ag) layers per source neutron was approximately 26 keV, which was larger than the energy deposited in the Hornyak button (approximately 5 keV). The results also indicate the neutron-detection efficiency saturates at just below 6.0% for a device with length larger than 20 cm. While better neutron-detection efficiency is expected from a longer detector, when selecting a length, one needs also to consider the size of SiPMs required, the overall space allocated for the detector and electronics, and the total cost of the resulting system.

![Neutron-detection efficiency](image_url)

Figure 5.3: Neutron-detection efficiency of the layered detector as a function of the detector length. The thicknesses of PMMA and ZnS(Ag) layers were set to 0.18 mm and 12 µm, respectively.
5.2.4 Gamma Rejection

The layered detector’s gamma-rejection capability was evaluated by determining the neutron-detection efficiency as a function of the background gamma-ray intensity (whereas for all baseline work, a background intensity of 10 gammas per neutron was assumed). A 5-cm long device with optimal layer thicknesses was used. As the number of gamma rays per neutron was increased, a higher LLD setting was required to achieve an S/N ratio of 100. Hence, the neutron-detection efficiency decreases, as shown in Fig. 5.4. For up to 40 gamma photons per event, this detector can achieve a neutron-detection efficiency larger than 1%.

![Graph showing neutron-detection efficiency vs. number of gamma rays per event]

Figure 5.4: A comparison of two new detectors’ gamma-rejection capabilities.

5.3 Homogenized Detector Results

5.3.1 ZnS(Ag) Fraction Optimization

The primary variable affecting the homogenized detector performance is the mass fraction of ZnS(Ag). A higher fraction produces but also absorbs more scintillation light. Figure 5.5 shows the impact of the ZnS(Ag) mass fraction for a 5-cm homogenized detector. At a mass fraction of 12%, a maximum neutron-detection efficiency of approximately 1.3% was
achieved.

5.3.2 Pulse Height Distributions

The pulse-height distribution and the associated neutron-detection efficiencies at different LLD settings of the best case are shown in Fig. 5.6. As also observed for the layered detector, Cherenkov noise can be readily rejected. At a LLD setting of 175 optical photons, the majority of the gamma-induced scintillation and Cherenkov noise can be discriminated to achieve an S/N ratio of 100, and the corresponding neutron-detection efficiency is about 1.3%.

![Figure 5.5: Impacts of the ZnS(Ag) mass ratio in the scintillation volume on neutron-detection efficiency.](image)

5.3.3 Length Evaluation

The homogenized detector’s efficiency as a function of detector length is shown in Fig. 5.7, for which the mass fraction of ZnS(Ag) was set to 12%. The results indicate the neutron-detection efficiency saturates at about 2.2%. To compare to the Hornyak button, at the length of one inch, the neutron-detection efficiency is about 0.8%. At this length, on average, one source neutron can result in approximately 12 keV deposited energy in the scintillator,
Figure 5.6: Performance of the 5-cm long, optimized homogenized detector.

which is larger than the 5 keV of the Hornyak button but less than the 26 keV of the layered detector.
5.3.4 Gamma Rejection

The homogenized detector’s gamma-rejection capability is illustrated in Fig. 5.4. Up to a gamma-to-neutron intensity ratio of about 20, this detector can achieve a neutron-detection efficiency above 1%. When the background exceeds 50 gamma rays per pulse event, the homogenized detector exhibits better performance than the layered detector. Hence, the homogenized detector is more resistant to gamma background, which may be explained by its overall lower efficiency.

5.4 Summary

Performance of the layered and the homogenized Hornyak-button variants was evaluated in Geant4. By collecting light at the transverse surfaces using SiPMs attached to the proposed devices, Cherenkov noise is reduced significantly, and gamma-induced scintillation and Cherenkov noise can be rejected by using simple pulse-height discrimination alone.

The improved light collection method allowed better scintillation volume designs for higher fast-neutron detection efficiency. For the same hodoscope-like conditions used to evaluate Hornyak button, at the length of 5 cm, the optimized layered detector was pre-
dicted to have an improved neutron-detection efficiency of approximately 3.3%, while the optimized homogenized detector was predicted to have an efficiency of approximately 1.3%. By increasing the detector lengths, efficiencies were shown to saturate at about 5.9% and 2.2% for the layered and homogenized devices, respectively. For more intensive gamma-ray background (gamma-to-neutron ratios above 50), the homogenized detector exhibited better performance than the layered detector.
Chapter 6

Fast-Sensitive MSNDs

Besides the Hornyak-button variants described in Chapter 5, fast-sensitive, actinide and hydrogenous MSNDs were also considered for the TREAT hodoscope. Fast-sensitive MSNDs are evolutions of well-established thermal-sensitive devices by using fast-neutron converters. Neutron converters considered are $^{237}$Np, $^{235}$U, natural uranium, and $^{232}$Th for actinide MSNDs and paraffin wax for hydrogenous MSNDs (H-MSNDs). Paraffin wax has a larger fission-spectrum-weighted macroscopic cross section than the actinide materials. However, actinide reactants allow higher LLD settings due to the large energy of fission fragments. In this chapter, these fast-sensitive MSNDs are evaluated using Geant4 and MCNP.

6.1 Description of the MSND

Shown in Fig. 6.1 is the basic design of an MSND [51]. The micro-structured trenches are etched into the high-resistivity $n$-type silicon substrate to a depth of 350 $\mu$m [70]. The $p$-type contacts are diffused along the trenches to form the $pn$ junction. Then, the trenches are backfilled with neutron converters. Finally, the ohmic contacts are added.

A neutron entering the detector has a certain possibility to interact with the converters in the trenches and to produce the charged particle(s). Then, the charged particle(s) might leave the trench and deposit energy in the silicon depletion region. This deposited energy can
excite electron-hole pairs. Under an applied bias, the motion of the charge carriers produces a detectable current. The resulting current can then be amplified, measured, and recorded by the counting electronics [71]. If the resulting current is beyond the LLD setting, a valid count is generated, and the neutron is detected.

Thermal-sensitive MSNDs have been developed at Kansas State University for decades [41]. Current generations of the thermal-sensitive devices use $^6$LiF to convert thermal neutrons. A typical MSND has 20-$\mu$m wide trench and 10-$\mu$m wall thickness [70]. At a length of 1 cm, it contains approximately 330 trench-wall pairs. The most-recent incarnation, known as the dual-sided MSND, has exhibited an intrinsic thermal neutron detection efficiency of 69% [42].

To adapt the existing MSND technique for the TREAT hodoscope, fast-sensitive, actinide and hydrogenous MSNDs were considered by using fast-neutron converters. The actinide MSNDs are loaded with $^{237}$Np, $^{235}$U, natural uranium, or $^{232}$Th. In a neutron event, one of the fission fragment pair may enter the active silicon region to generate signal. The H-MSNDs use paraffin wax to convert fast neutrons. The recoil proton from neutron scattering reaction with the hydrogen nuclide may enter the depleted silicon region to liberate electron-ion pairs.
6.2 Cross Section Comparison of the Converters

Efficiency of a fast-sensitive MSND depends on the probability that a fast neutron interacts with the converter. Shown in Fig. 6.2 are the microscopic cross sections of the converting reactions and the Watt fission spectrum \( \chi(E) \) of neutrons from \( ^{235}\text{U} \) thermal fission reaction (as shown in Eq. (4.1)). As a comparison, the microscopic cross section of the \( ^{6}\text{Li}(n, \alpha)^{3}\text{H} \) reaction at 0.025 eV is 937 b, as shown in Table 2.1. The \( \chi \) spectrum peaks at the most-probable neutron energy of approximately 0.74 MeV and leads to an average neutron energy of about 2 MeV.

\[
\bar{\sigma} = \frac{\int \sigma(E)\chi(E)dE}{\int \chi(E)dE}, \quad (6.1)
\]

where the integrals are from \( 10^{-11} \) to 20 MeV, and the results are shown in Table 6.1. Paraffin wax has the highest macroscopic cross section of 0.32 cm\(^{-1}\), and \( ^{237}\text{Np} \) has the largest cross section among actinides by a small margin. While the neutron-converting probabilities of

Figure 6.2: Microscopic cross sections of the target reactions [12] and the \( ^{235}\text{U} \) Watt fission spectrum by thermal neutron.

To quantify the probabilities of the fission neutrons interacting with the nuclides, the fission-spectrum-weighted microscopic cross sections were computed as
the actinide MSNDs are smaller than the H-MSNDs, the actinide MSNDs allow higher LLD settings to reject neutron-activation gamma rays in the hodoscope because of the large energy of fission fragments.

Table 6.1: Comparison of the converter cross sections.

<table>
<thead>
<tr>
<th>Converter</th>
<th>Density (g/cm³)</th>
<th>Molecular weight (g/mole)</th>
<th>$\overline{\sigma}$ (b)</th>
<th>$\Sigma$ (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>paraffin wax (C_{25}H_{52} [72])</td>
<td>0.93</td>
<td>352.68</td>
<td>3.93</td>
<td>0.32</td>
</tr>
<tr>
<td>$^{237}$Np</td>
<td>20.25</td>
<td>237.05</td>
<td>1.31</td>
<td>0.067</td>
</tr>
<tr>
<td>$^{235}$U</td>
<td>18.95</td>
<td>235.04</td>
<td>1.21</td>
<td>0.059</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>18.95</td>
<td>238.05</td>
<td>0.31</td>
<td>0.015</td>
</tr>
<tr>
<td>$^{232}$Th</td>
<td>11.72</td>
<td>232.04</td>
<td>0.075</td>
<td>0.0023</td>
</tr>
</tbody>
</table>

6.3 Modeling Details

The fast-sensitive MSNDs were evaluated using Geant4 and MCNP. A previous MCNP6 simulation showed the $^{237}$Np-filled and the $^{235}$U-filled MSNDs yielded efficiencies larger than 1% [43]. In the following, the actinide MSNDs filled with $^{235}$U, natural uranium, and $^{232}$Th were re-evaluated in Geant4 using the fission fragment generator (FFG) [34]. The FFG samples and tracks fission fragments in a single run to simplify the two-step evaluation in MCNP6 [43].

$^{237}$Np-filled MSNDs were not evaluated because Geant4 does not include the neutron data for $^{237}$Np [73]. Though absent, the predicted efficiencies of the $^{237}$Np-filled MSNDs were better than those of $^{235}$U-filled devices [43]. More importantly, $^{237}$Np may be preferred to $^{235}$U because it is insensitive to neutrons below about 1 MeV, which are generated by the slowing down of the fast neutrons in the test section [11] and the collimator in the TREAT facility. These sub-fast neutrons are a further source of background radiation in addition to neutron-activation gamma rays.

The neutron event pulse-height distributions (NEPHDs) of the H-MSNDs were computed in Geant4 and MCNP6 for comparison. The pulse-height distributions (PHDs) of the H-MSNDs from hodoscope-like gamma rays were calculated in Geant4, where the number of
source particles per event was adjustable to simulate the gamma ray strength. For completeness, the neutron-detection efficiencies of the H-MSNDs at the 300-keV LLD [71] and the LLD settings that achieved S/N ratio of 100 based on the gamma event PHDs were reported, respectively.

6.3.1 Neutron Data Library

Performance of fast-sensitive MSNDs was evaluated in Geant4 10.03.p01 [32] and MCNP6.1 [33]. The G4NDL4.5 neutron data library [73] was employed in the Geant4 calculations. This library is primarily based on the ENDF/B-VII.1 nuclear data [12]. Because the G4NDL4.5 library only contains the data for isotopes up to uranium [73], the $^{237}$Np-filled MSNDs were not evaluated with Geant4. The MCNP6 calculations used the ENDF/B-VII.0 nuclear data [74]. All cross sections used were for a temperature of 293 K.

6.3.2 MSND Models for NEPHDs

Shown in Fig. 6.3 and Fig. 6.4 are the MSND models developed for NEPHDs in Geant4 and MCNP6, respectively. Because the neutron-sensitive materials in the MSNDs are primarily the converters in the trenches, these models consisted of the etched silicon region, i.e., the repeated trench-wall structures, as shown in Fig. 6.5. For illustration, the trench and the wall widths in Fig. 6.3 and Fig. 6.4 were 0.1 cm. The NEPHDs of the actinide MSNDs were computed in Geant4 using the FFG. The NEPHDs of the H-MSNDs were computed in Geant4 and MCNP6 for comparison.

6.3.3 MSND Model for Gamma Event PHDs

Shown in Fig. 6.6 is the H-MSND model to compute the gamma event PHDs in Geant4. In the model, the electronic board, the bulk silicon region, and the etched silicon region were considered. Their dimensions in the height-depth plane are shown in Figure 6.5. These volumes were sensitive to the gamma rays due to the relatively high-Z materials. Silicon has
an atomic number $Z$ of 14, and the electronic board contained copper ($Z = 29$) and bromine ($Z = 35$).

Geant4 was used to compute the gamma event PHDs because the number of source particles in a pulse event was adjustable [60]. Hence, specific gamma-to-neutron intensity ratio can be sampled to simulate the hodoscope environment.

Based on the Geant4-computed neutron and gamma event PHDs of the H-MSNDs, LLDs that achieved S/N ratio of 100 [69] were set to define the practical neutron-detection efficiencies in the hodoscope. The actinide MSNDs' responses to the gamma rays were not evaluated because the energetic fission fragments allowed high LLD settings intrinsically.
Figure 6.4: The developed MSND model for NEPHDs in MCNP6. The trench (T) and wall (W) widths were 0.1 cm for illustration.

6.3.4 Physics Settings

Geant4 Physics Setting

The QGSP BERT HP reference physics list [55] was used in the Geant4 calculations. In Geant4, the secondary particle production threshold is specified as the range cutoff in distance unit [60], i.e., the secondary particle that can travel longer than the cutoff is generated.
Figure 6.5: The etched silicon region was modeled to compute the NEPHDs in Geant4 and MCNP6. To evaluate the H-MSNDs’ responses to the gamma rays in Geant4, the bulk silicon region and the electronic board were added. The neutron and the gamma source generation planes were set correspondingly.

Figure 6.6: The H-MSND model to calculate the gamma event PHDs in Geant4.
Based on the range cutoff, the production threshold energies for different materials are computed. The energy equivalences of the range cutoff cannot be lower than a lower-bound, threshold value; otherwise, the lower-bound value will be used. For best accuracy, the lower-bound value was set to 250 eV, which is the lower limit for the low-energy electromagnetic processes [32], and the range cutoff was set to 10 nm to activate the lower-bound value. In addition, the produced particles are tracked to zero energy [60].

**MCNP6 Physics Setting**

In MCNP6, to obtain the most accurate energy deposition, the potential secondary particles (proton, heavy ion, photon, and electron) were transported in the calculations [35]. In the neutron physics card, the analog energy limit parameter, emcnf, was set to 100 MeV. This setting performed analog capture for the neutrons with energies smaller than 100 MeV, which provided reliable f8 pulse-height tally. The light-ion and heavy-ion recoil and neutron capture ion algorithm (NCIA) control parameter, coilf, was set to the recommended value of four [35], which generated one ion from neutron elastic scattering. In the proton physics card, the recl light ion recoil control parameter was set to one. Hence, one light ion was created at each proton elastic scatter event with light nuclei, i.e., hydrogen, deuteron, triton, $^3$He, and $^4$He. The default values for the other physics settings were used. The default energy cutoffs for neutron (0), electron (1 keV) and photon (1 keV) were used. The energy cutoffs for the proton and heavy ion were decreased to the lower limit of 1 keV.

### 6.3.5 Source Terms

**Neutron Source**

In the NEPHD calculations, mono-directional source neutrons traveled along the length-wise direction. The neutron trajectories in Geant4 are shown in Fig. 6.3. These neutrons were generated uniformly in the depth-height plane of the etched silicon region, as shown in Figure 6.5. Energies of the neutrons were sampled from Eq. (4.1).
Gamma-Ray Source

Details of the gamma source are specified in Section 4.2, i.e., fission-spectrum gamma rays were shot into the detector isotropically with an intensity of 10 gamma rays per neutron. Because the gamma rays may interact within the electronic board and the silicon substrate, the source gamma rays were born in a plane covering the H-MSND (2.4 cm × 1.5 mm, Figure 6.5). Considering the different sampling areas of the neutron and the gamma sources (Figure 6.5), to maintain an intensity of 10 gamma rays per fast neutron, the number of gamma rays per event \( N_g \) was scaled to

\[
N_g = \frac{A_g}{A_n} \times 10 = \frac{2.4 \times (0.1 + 0.05)}{2 \times 0.035} \times 10 \approx 51,
\]

where \( A_g \) and \( A_n \) are the areas of the gamma-ray and the neutron source planes, respectively.

6.3.6 Tally Methods

In the NEPHD calculations, the deposited energy spectra in the walls were tallied. In the gamma event PHD calculations, the deposited energy spectra in the silicon depletion region, i.e., the walls and the bulk silicon, were tallied.

In Geant4, the deposited energy spectra were computed by the user actions [60]. In MCNP6, the f6 tally by all the tracked particles was first used to compute the deposited energy in the tally region. Then, based on the f6 tally, the PHD was computed by the \( ft \, phl \) option of the f8 tally [35].

6.4 Assumptions of the Modeling

To evaluate the MSNDs, a few assumptions were made:

1. The neutron interactions outside the etched silicon region, e.g., the bulk silicon region, were not considered, though these reactions may contribute to the neutron detection efficiency.
2. A perfect charge collection efficiency in silicon was assumed. Indeed, the charge collection efficiency may deteriorate due to the damage or degradation of silicon caused by the fission fragments or protons. These negative effects need further experimental evaluation.

3. The neutrons traveled along the detector length direction perfectly. The impact of any departure from this idealized alignment in practical applications warrants future consideration.

6.5 Evaluation and Results

6.5.1 Effects of Parameters

The fast-sensitive MSNDs with different trench widths, wall widths, and lengths were evaluated. All the detectors had 350-µm depth and 2-cm height. The depth and height were consistent with the current thermal-sensitive MSNDs [70].

For a fixed length, when the trench width is small, an increase of the trench width results in higher neutron-sensitive volume fraction for better efficiency. If the trench width increases further, more charge particles are generated, but a large portion of their energies are deposited in the trenches. Because the electric signal is caused by the energy deposited in the silicon, trapping of the charge particles in the trenches deteriorate the efficiency.

A wider wall enables the charged particles to deposit more energy in the silicon, which allows a higher LLD setting. However, for a fixed length, a wider wall leads to smaller neutron-sensitive volume fraction. Therefore, fewer charged particles are generated. Additionally, a wider wall increases the H-MSND’s gamma sensitivity.

For fixed trench and wall widths, a longer MSND yields better efficiency because the neutron penetrates more trench-wall pairs. Longer lengths can be achieved by stacking the processed silicon substrates into an array, similar to proposed $^3$He replacement devices [75]. The length is also limited by the space in the hodoscope to install the MSND, i.e., approximately 20 cm.
6.5.2 Actinide MSNDs

Trench-Wall Optimization

Shown in Fig. 6.7 are the Geant4-computed neutron detection efficiencies of the 2-cm long $^{235}\text{U}$-filled MSNDs with different trench and wall widths at a LLD setting of 5 MeV. With 20-µm trench and 10-µm wall widths, the $^{235}\text{U}$-filled MSND yields intrinsic neutron detection efficiency of about 1.2%. Though better efficiencies are achievable with smaller trench widths, filling the trenches with uranium has proven difficult [43].

![Graph showing neutron detection efficiencies with varying trench and wall widths.]

Figure 6.7: The Geant4-computed neutron-detection efficiencies of the 2-cm long $^{235}\text{U}$-filled MSNDs with different trench and wall widths at the 5-MeV LLD.

NEPHDs

The Geant4-predicted distributions of the energy deposition by the fission fragments in silicon of the actinide MSNDs with 2-cm length, 20-µm trench and 10-µm wall widths are shown in Figure 6.8. The distribution of the $^{235}\text{U}$-filled MSND features peaks A and B at about 18 MeV and 30 MeV, respectively, plateaus C and D, and slopes E and F. The features for MSNDs filled with natural uranium and $^{232}\text{Th}$ are not significant (probably also exist).

The formation of these features may be explained using Fig. 6.9, where P1, P2, and P3 are extreme paths for a fission fragment to enter the silicon wall. P1 is the shortest length to...
penetrate the wall along the depth direction. P2 is nearly perpendicular to the wall depth direction. P3 represents the path for a fission fragment to deposit all kinetic energy while reaching the wall width limit.

While the true fission-fragment distribution was sampled by the fission fragment generator in Geant4 to generate the results in Fig. 6.8, to understand the features exhibited in Figure 6.8 in more depth, consider a representative fission fragment pair of $^{95}$Sr and $^{139}$Xe with initial kinetic energies of 100 and 70 MeV, respectively. In the uranium trench, the projected ranges for these two ions are 5.7 and 4.1 $\mu$m, respectively, and in the silicon wall, the projected ranges for these two ions are 16.7 and 11.8 $\mu$m, respectively [39]. Based on the projected ranges in uranium and 20-$\mu$m trench, only one fission fragment of a pair can enter the wall.

If a fission fragment enters the wall with energy not sufficient to leave the wall even along the shortest path P1, the contribution of this fission fragment is under peak B for Sr, or peak A for Xe.

If a fission fragment enters the wall with more energy to penetrate the wall along the shortest path P1, and its path is between P2 and P3, all of its kinetic energy is deposited in the wall because the 2-cm height and 350-$\mu$m etch depth (as shown in Fig. 6.5) are much larger dimensions than the 10-$\mu$m wall width. If the fission fragment is Sr, its deposited energy is 100 MeV less the energy deposited in the born trench 1, which leads to slope F in Fig. 6.8. If the fission fragment entering the wall is Xe, the corresponding feature is slope E.

If the range of the fission fragment that enters the wall is larger than P1, and the path is between P3 and P1, a part of the kinetic energy is deposited in the wall. If the fission fragment is Sr, the contribution is under the area of plateau C, slope E, and plateau D with height of plateau D. If the fission fragment is Xe, it contributes to plateau C besides the contribution of Sr.

The results in Fig. 6.8 indicate the actinide MSNDs allow high LLD settings, e.g., 10 MeV.
Figure 6.8: The Geant4-predicted distributions of the energy deposition in silicon by fission fragments of the 2-cm long actinide MSNDs with 20-µm trench and 10-µm wall widths.

Figure 6.9: Extreme paths of fission fragments in the actinide MSND.

**Efficiencies of the Actinide MSND Arrays**

With 20-µm trench and 10-µm wall widths, intrinsic neutron detection efficiencies of the actinide MSNDs with different lengths are shown in Figure 6.10. The 5-MeV LLD was applied. The $^{235}$U-filled MSNDs with lengths larger than 14 cm yield intrinsic neutron detection efficiency of about 2.6%. The MSNDs filled with natural uranium and $^{232}$Th cannot achieve efficiencies larger than 1%.
Figure 6.10: The Geant4-computed intrinsic neutron detection efficiencies of the actinide MSND arrays. The MSNDs had 20 µm trench and 10 µm wall widths. The LLDs were set to 5 MeV.

**Comparison between Geant4 and MCNP6**

The Geant4-computed and the MCNP6-computed total deposited energies in the trenches per neutron of the actinide MSNDs were compared. The MSNDs had the geometry of 2-cm length, 20-µm trench, and 10-µm wall widths (orientation of the dimensions is shown in Fig. 6.1). This particular comparison was made because MCNP6 assumes the fission energy is deposited locally [35]. To be consistent, the FFG in Geant4 was turned off.

Shown in Table 6.2 are the computed results, which agree relatively well. The difference is computed by

\[ E_g - E_m, \]  

(6.3)

where \( E_g \) is the Geant4-predicted deposited energy, and \( E_m \) is the calculated deposited energy by MCNP. For \(^{235}\text{U}\), the Geant4-computed tally is smaller than the MCNP6 value by about 0.073 MeV. The differences might be caused by the different cross section libraries used by the two codes, as discussed in Section 6.3.1.
Table 6.2: Total deposited energies (MeV) in the trenches per neutron computed by Geant4 and MCNP6 and their differences (relative to MCNP6).

<table>
<thead>
<tr>
<th>Reactant</th>
<th>MCNP6</th>
<th>Geant4</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}$U</td>
<td>10.44 ± 0.020</td>
<td>10.37 ± 0.041</td>
<td>−0.073 ± 0.045</td>
</tr>
<tr>
<td>Natural Uranium</td>
<td>2.75 ± 0.012</td>
<td>2.64 ± 0.021</td>
<td>−0.11 ± 0.024</td>
</tr>
<tr>
<td>$^{232}$Th</td>
<td>0.46 ± 0.0022</td>
<td>0.42 ± 0.0080</td>
<td>−0.031 ± 0.0083</td>
</tr>
</tbody>
</table>

### Alpha Decay of the Reactants

Besides the necessity of discriminating gamma rays in the hodoscope environment, the LLD of the actinide MSNDs must be set to account for the decay alpha particles of the converters. Table 6.3 summarizes the alpha decay information of the actinide reactants in the MSNDs with the geometry of 2-cm length, 20-µm trench, and 10-µm wall widths. The energies of the alpha particles are approximately 4 MeV. In the 10-µs pulse shaping time of current MSND [71], the number of alpha particles would not exceed 1.41. Hence, a 5-MeV LLD should be sufficient to reject the alpha particles and the gamma rays. In addition, based on the NEPHDs (Fig. 6.8), the LLD can be set to 10 MeV without significant efficiency deterioration.

Table 6.3: Alpha decays of the 2-cm long actinide MSNDs with 20-µm trench and 10-µm wall widths. Data from Ref. [16].

<table>
<thead>
<tr>
<th>Reactant</th>
<th>Half life (s)</th>
<th>Number of α particles in 10 µs</th>
<th>Most-probable α energy (MeV) (abs. %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}$U</td>
<td>2.22 ×10$^{16}$</td>
<td>1.41</td>
<td>4.40 (57.73)</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>1.41 ×10$^{17}$</td>
<td>0.22</td>
<td>4.20 (79.00)</td>
</tr>
<tr>
<td>$^{232}$Th</td>
<td>4.42 ×10$^{17}$</td>
<td>0.045</td>
<td>4.01 (78.20)</td>
</tr>
</tbody>
</table>

### 6.5.3 Hydrogenous MSNDs

#### Trench-Wall Optimization at 300-keV LLD

At 300-keV LLD, the intrinsic neutron detection efficiencies of the 2-cm long H-MSNDs with different trench and wall widths were computed in Geant4 and MCNP6, and the results are shown in Fig. 6.11. Results of the two codes agree well, and the slight differences may be
caused by the different cross-section libraries (Section 6.3.1). With 20-µm trench and 10-µm wall widths, the efficiency of about 10% was predicted.

Figure 6.11: The Geant4- and MCNP6-computed intrinsic neutron detection efficiencies of the 2-cm long H-MSNDs with different trench and wall widths. A 300-keV LLD was set.
NEPHDs at 300-keV LLD

Shown in Fig. 6.12 are the Geant4- and MCNP6-computed NEPHDs of the 2-cm H-MSND with 20-µm trench and 10-µm wall widths. On average, about half of the neutron energy is transferred to the recoil proton. Because the most-probable energy of fission-spectrum neutrons is about 1 MeV, the corresponding proton energy is about 500 keV, and, hence, a peak at about 500 keV exists. Because the energy distribution of the recoil proton is relatively uniform from the neutron energy to zero, in the lower part of the curve, protons from more higher-energy neutrons can contribute, and, hence, the distribution accumulates in the low energy part.

Figure 6.12: The Geant4- and MCNP6-computed NEPHDs of the 2-cm long H-MSND with 20-µm trench, 10-µm wall widths.

Efficiencies of the H-MSND Array at 300-keV LLD

With 20-µm trench and 10-µm wall widths, the Geant4- and MCNP-computed intrinsic neutron detection efficiencies of the H-MSNDs with different lengths are shown in Figure 6.13. A 300-keV LLD was applied. The efficiency saturates at about 26%.
Figure 6.13: The Geant4- and MCNP6-computed neutron detection efficiencies of the H-MSNDs with different lengths. The 300-keV LLD was set. The H-MSNDs were with 20-µm trench and 10-µm wall widths.

**Trench-Wall Optimization at S/N 100**

Table 6.4 summarizes the trench and wall widths of the 2-cm long H-MSNDs that yielded intrinsic neutron detection efficiencies larger than 2%. The LLDs were set to achieve an S/N ratio of 100 based on the neutron and the gamma event PHDs computed by Geant4. The H-MSND with 60-µm trench and 40-µm wall widths yields the best efficiency of 2.47%, where the 1.2-MeV LLD is set to achieve an S/N ratio of 100.

Table 6.4: The trench and wall widths of the 2-cm long H-MSNDs that yielded neutron detection efficiencies (in percent) above 2% at the LLD settings that achieved S/N ratio of 100. The LLD settings in MeV are shown in the parentheses.
Neutron and Gamma Event PHDs at S/N 100

Figure 6.14 shows the Geant4-computed neutron and gamma event PHDs of the 2-cm long H-MSND with the optimized 60-\(\mu\)m trench and 40-\(\mu\)m wall widths. The peak of the NEPHD is beyond 1 MeV.

![Figure 6.14: The Geant4-computed neutron and gamma event PHDs of the 2-cm long H-MSND with 60-\(\mu\)m trench and 40-\(\mu\)m wall widths.](image)

Efficiencies of the H-MSND array at S/N 100

With 60-\(\mu\)m trench and 40-\(\mu\)m wall widths, the neutron-detection efficiencies of the H-MSNDs with different lengths are shown in Fig. 6.15. The LLDs were set to achieve S/N ratio of 100. The maximum efficiency of about 9.6% is predicted at the length of 20 cm.

6.6 Summary

Performance of the actinide MSNDs and the H-MSNDs for the TREAT hodoscope was evaluated in Geant4 and MCNP6. The actinide MSNDs allow high LLD settings due to the energetic fission fragments, while paraffin wax in the H-MSNDs leads to more fast neutron interactions.
Actinide MSNDs filled with $^{235}\text{U}$, natural uranium, and $^{232}\text{Th}$ were evaluated in Geant4 using the fission fragment generator. With the LLD set to 5 MeV, the intrinsic neutron-detection efficiency of the $^{235}\text{U}$-filled MSNDs was 1.2% for a 2-cm device length and saturated at 2.6% for lengths beyond 14 cm, where 20-µm trench and 10-µm wall widths were assumed. The deposited energy in $^{235}\text{U}$ predicted by Geant4 was smaller than the MCNP6-predicted value by about 0.073 MeV. The efficiencies of the $^{235}\text{U}$-filled MSNDs acted as the lower limits of the $^{235}\text{Np}$-filled devices, which are preferred due to their insensitivity to the slow neutrons. The MSNDs filled with natural uranium and thorium were predicted to have efficiencies lower than the 1%.

With the LLD set to 300 keV, Geant4 and MCNP6 predicted an efficiency of about 10% for a 2-cm long H-MSND with 20-µm trench and 10-µm wall widths and an efficiency of about 26% for a detector length of 20 cm. For an LLD set to achieve an S/N ratio of 100 when including gamma-ray noise, the best-case, Geant4-predicted efficiencies were 2.5% and 9.6% for 2-cm and 20-cm long devices with 60-µm trench and 40-µm wall widths.
Chapter 7

Micro-Pocket Fission Detectors

Micro-Pocket Fission Detectors (MPFDs) are in-core neutron detectors for TREAT, which can be operated in pulse mode and use the large amount of deposited energy by the fission fragments to separate neutron pulses from other in-core radiation. While for the largest TREAT transients, i.e., neutron flux in the order of $10^{17} \text{ cm}^{-2}\text{s}^{-1}$, the pulse mode may not be suitable due to the dead time count loss, the electron collection process in the MPFDs still needs to be quantified to interpret the measurements and to optimize future designs. In this chapter, a Garfield-based computational tool is explored to evaluate the electron motion in MPFDs, and the gained experiences in the modeling process are detailed. Preliminary results of the MPFD evaluation are presented.

7.1 MPFD Physics

The schematic of the MPFD developed for Idaho National Laboratory is shown in Fig. 7.1. It is a miniature fission chamber designed to monitor the neutron flux at a point inside the core. The chamber is typically filled with argon gas at a pressure of 30 psig (or 3.04 atm), and in this work, a gas temperature of 50 °C was assumed. Two electrode wires, each with a diameter of 0.255 mm, penetrate the gas volume to create electric field. A thin, fissile layer is deposited in the gas volume to convert in-core neutrons. A typical thickness of the fissile
layer is in the nm range [46] and can be adjusted for different applications.

In a neutron event, one nucleus of the fission fragment pair enters the gas and deposits approximately a few MeV of energy. Along the path of the fission fragment, ionized electron-ion pairs are generated. The charge carriers are drifted under applied electric field and, at the same time, diffuse. The motion of the charge carriers induces current in the external circuit, which is processed to generate a pulse.

The electron collection process in MPFDs needs to be quantified to assist the development. Because electrons move thousands of times faster than ions, pulse-mode MPFDs are usually connected to an $RC$ circuit to truncate the signal after electrons are collected. Therefore, the time to collect electrons from a neutron pulse event needs to be determined in order to select a suitable $RC$ circuit. In addition, pulse-mode detectors are designed to minimize dead time count loss. Ideally, the electrons from one neutron event are collected, and the signal is processed before the next neutron event occurs. To accommodate a range of in-core neutron flux levels, the reaction rate of the neutron-converting, fission reaction can be adjusted by changing the thickness of the fissile layer. A faster electron collection allows a thicker fissile layer to produce higher count rate while maintaining a small dead time, which reduces the relative error. Overall, the thickness of the fissile layer, the speed of the electron collection, and the electronics system need to be matched to achieve optimal performance in TREAT and other reactor cores.

### 7.2 Computational Scheme

To simulate the electron collection process in MPFDs, a Garfield-based, computational scheme [76] was used, as shown in Fig. 7.2. The scheme consists of the following codes: Garfield++ (version v1r0)[36], Gmsh (version 3.0.6) [37], Elmer (version 8.3) [38], and stopping and range of ions in matter (SRIM) (version 2008.04) [39].

Gmsh was used to construct the gas volume (shown in Fig. 7.1) and to generate the finite-element mesh for Elmer. The Gmsh output was converted to Elmer-suitable format using the **ElmerGrid** module, and the electric field was calculated by the **ElmerSolver** module.
using a finite-element method. The Elmer outputs were imported into Garfield++ via the ComponentElmer class.

SRIM was used to generate the energy loss tables of a pair of representative fission fragments, $^{95}_{38}$Sr and $^{139}_{54}$Xe. These tables were imported into Garfield++ using the TrackSrim class.

With the inputs from Elmer and SRIM, Garfield++ simulated the ionization of fission fragments in gas and created electron clusters along its path based on the deposited energy and the user-supplied work function (Eq. (2.11)) and fano factor (Eq. (2.12)) of the gas. Then, the drift of the electrons in the clusters under the Elmer-computed electric field and the diffusion process were simulated in Garfield++ using algorithms based on the Monte Carlo method. During the electron transport, the induced current generated by the electron movement was calculated simultaneously using the Shockley-Ramo theorem.
Figure 7.2: The computational scheme to evaluate MPFDs.

7.3 Gmsh

7.3.1 Running Modes

Gmsh is an open-source, three-dimensional (3-D) finite-element grid generator with a built-in CAD engine and postprocessor. Gmsh can be run in an interactive graphical user interface (GUI) mode or the non-interactive batch mode. The GUI mode is useful to examine the geometry and the mesh quality. The GUI mode is built on the Fast Light Toolkit (FLTK) [77] configured with OpenGL support. Thus, to enable the GUI mode, the FLTK module needs to be pre-installed, and the Gmsh source code needs to be compiled with the GUI-support options on.

The GUI mode greatly facilitates model construction. Geometry entities can be added to the model easily through the GUI interface, and the software automatically adds the corresponding Gmsh commands to the underlining plaintext .geo script.

However, the GUI mode is limited in that it does not support all the Gmsh commands. For full functionality, batch mode must be used instead. To build the model in batch mode, Gmsh uses C++-like commands, which are hard coded by the user in the geo text file. In particular, the batch mode supports user-defined functions, loops, and if conditions, which are useful for parameterization. In this study, both modes were used.
### 7.3.2 Geometry Construction

The geometry modeling in Gmsh consists of the elementary and the physical entities. To define the elementary geometry, Gmsh provides the basic built-in and the more advanced OpenCASCADE geometry kernels. The two kernels are not fully compatible, and, hence, it is recommended to build the model using either of the kernels, which is specified by the `SetFactory` command. The built-in kernel builds the geometry in a bottom-up flow by successively defining points, lines (by connecting points), surfaces (by line loops), and volumes (by surface loops).

The more advanced OpenCASCADE kernel was used to construct the MPFD geometry shown in Fig. 7.1. To enable the kernel, the *Open CASCADE* software [78] needs to be pre-installed. This kernel implements constructive solid geometry and provides additional commands to define lines, surfaces, volumes, and boolean operations that are not available in the built-in kernel. Specifically, standard volumes can be directly defined using the OpenCASCADE kernel. If a volume is defined in this way, Gmsh still implicitly constructs the underlying points, lines, and surfaces that form the volume to mesh the geometry. The identification numbers of these underlying geometry entities can be found by using the GUI mode and are needed to define the characteristic length as discussed below. The non-standard volumes can be defined through line loops using the ThruSections command in the OpenCASCADE kernel.

When an elementary point is defined explicitly, the mesh element size at the point can be specified via the characteristic length input parameter at initialization. For the points that are implicitly constructed, this parameter can be specified using the Characteristic Length function using the associated identification numbers found using the GUI mode.

The physical entity is a group of elementary geometry entities. While not required, physical entities are defined to facilitate the mesh generation in Gmsh. If defined, the output mesh only contains the elements that belong to the physical entities. In addition, the physical entities bridge Gmsh and Elmer. When the Gmsh output is imported into Elmer to calculate the electric field, the physical surface defined in Gmsh corresponds to the target
boundaries entity in Elmer to apply boundary condition. The physical volume corresponds to the body entity in Elmer to specify governing equation and to define the material relative permittivity (or dielectric constant).

### 7.3.3 Geometry Meshing

Gmsh generates a mesh from the bottom up. Lines are discretized first, and, then, the line mesh is used to mesh the surfaces. Finally, the surface mesh is used to mesh the volumes. The *unstructured* or the *structured* meshing algorithms for 3-D geometry are provided. The unstructured algorithms generate tetrahedra, while the structured algorithms generate tetrahedra, hexahedra, prisms or pyramids depending on the type of the surface meshes.

The Delaunay (which is the default) and the Frontal 3-D unstructured meshing algorithms are implemented, and the quality of the elements produced by the two algorithms are comparable [79]. Other mesh algorithms exist that are not fully documented in the Gmsh reference manual [79]. For instance, the Delaunay, New Delaunay, Frontal, Frontal Delaunay, Frontal Hex, MMG3D, and R-tree mesh algorithms can be selected via the *Mesh.Algorithm3D* option. The del3d, front3d, mmg3d, and pack mesh algorithms can be specified in the command line via the *algo* option. The unspecified mesh algorithms may be the structured type or in the experimental phase. In addition, the built-in and the Netgen algorithms are provided to optimize the mesh quality.

The size of the mesh elements can be defined in three ways. The first is from the characteristic lengths of the elementary points. If the *Mesh.CharacteristicLengthFromCurvature* option is set, the mesh is adapted with respect to the curvature of the geometrical entities. Finally, the size can also be specified by defining fields. These three methods can work simultaneously. In this case, the smallest element size is selected at any given point. The first two methods were used in this work.
7.3.4 MPFD Gmsh Model

In this work, the OpenCASCADE kernel was used to model the MPFD geometry shown in Fig. 7.1. The global gas volume was constructed using the ThruSections command by defining the top and the bottom line loops. The two wire volumes were constructed by the Cylinder command, and, then, the two wire volumes were subtracted from the global gas volume using the difference boolean operation. The resulting gas volume was set as a physical volume. This physical volume was later used in ElmerSolver to assign governing equation and the relative permittivity of argon gas. The cylinder surfaces of the two wire volumes were set as two physical surfaces, respectively. The physical surfaces were used in ElmerSolver to specify boundary condition, i.e., to apply voltage on the electrodes. The default Delaunay mesh algorithm and the built-in mesh-optimize algorithm were used to mesh the geometry.

The characteristic length of 0.02 was applied to all the elementary points to produce elements with sufficient quality required by Garfield++. Because the elementary points associated with the wire volumes were created implicitly by Gmsh, the Characteristic Length function was used to set the value of 0.02 at these points, whose identification numbers were found using the GUI mode. The Mesh.CharacteristicLengthFromCurvature option was set.

With all the commands written in a geo file, Gmsh was run with the -3 -order 2 command line options to generate a 3-D mesh with second-order tetrahedral elements. The second-order elements are supported in Garfield++. A msh file was generated to describe the meshed geometry. The meshed geometry of the MPFD is shown in Fig. 7.3.

7.4 Elmer

The Gmsh-generated msh file was used in Elmer to calculate the electric field. Elmer is an open-source, finite-element software package for the solution of partial differential equations. It consists of several modules, and the the ElmerGrid and the ElmerSolver modules were
used in this study.

### 7.4.1 ElmerGrid

ElmerGrid was used to convert the msh file to the format readable for ElmerSolver. The command used was

```
ElmerGrid 14 2 GmshFile.msh -autoclean.
```

The option 14 indicated the input is from Gmsh, and the option 2 stated the output is for ElmerSolver. GmshFile.msh was the mesh file generated by Gmsh. The autoclean flag re-numbered the physical surfaces and the physical volumes defined in Gmsh starting at one and with unit increment following the defining sequence. The physical surfaces and the physical volumes are re-numbered independently. Hence, the identification number of the defined physical gas volume in Gmsh was re-set to one, and this physical volume corresponded to body 1 in ElmerSolver to specify the governing equation and dielectric constant of argon gas. The identification numbers of the two wire physical surfaces were re-numbered to one and two, respectively. These two physical surfaces corresponded to target boundaries 1 and 2 in ElmerSolver, respectively, to assign specific boundary condition, i.e., applying different voltages on electrodes.
After applying the aforementioned command, ElmerGrid created a subdirectory containing the generated mesh.boundary, mesh.elements, mesh.header, and mesh.nodes files.

### 7.4.2 ElmerSolver

ElmerSolver reads a text sif file, which specifies the location of the ElmerGrid outputs, the applied voltages at the electrodes via the target boundaries keyword, the relative permittivity of argon gas, the electrostatic solver to calculate the electric field, the assignment of the governing equation, and the material properties of the gas body. The used sif file is shown in Appendix B.

Two electric field maps were generated, in which 100-V and 1-V voltages were applied to anode wire, respectively, and the cathode was grounded. The field map with 100-V bias on anode was used in Garfield++ to drift electrons, and the map with 1-V anode was the weighting field to calculate the induced current used in the Shockley-Ramo theorem. The calculated field maps were written in the generated result files.

Shown in Fig. 7.4 is the Elmer-computed electric field inside the gas volume with 100-V bias on the anode wire. The plot was generated in Garfield++ using the ViewField class. The maximum magnitude is about 900 V/cm near the electrode wires. Shown in Fig. 7.5 is the weighting field, which has the same shape as Fig. 7.4.

### 7.5 Garfield++

Garfield++ is a toolkit written in C++ mainly used to simulate the electron transport in gaseous detectors. The electron transport properties in gas mixtures under different electric and magnetic fields are calculated by the built-in interface to the Magboltz program [45], and the computed properties in argon gas were validated against experimental values [80]. In particular, the Magboltz-predicted electron drift speed was compared to an analytic approximation, and the details can be found in Appendix C. The main code structure of a Garfield++ application is shown in Fig. 7.6.
The MediumMagboltz class was used to define the argon gas at a pressure of 30 psig and a temperature of 50 °C. The density of argon gas at this condition was calculated automatically by Garfield++ using the ideal gas law.

The electron transport properties in gas are computed by the underlying Magboltz...
program. If the electrons are tracked by the Monte Carlo integration algorithm, an electron transport table needs to be calculated using the `GenerateGasTable` function in the `MediumMagboltz` class. This table provides the drift velocity, longitudinal and transverse diffusion coefficients, attachment and Townsend coefficients of electron tracking in the defined gas as a function of electric and magnetic fields. In this study, no magnetic field existed, and, thus, the generated table was one-dimensional and solely depended on electric field.

To generate the table, the range of the electric field, the number of grid points spanning the electric-field range, and the number of electron collisions inside the gas need to be specified. Because it is time-consuming to generate the table, in this work, a coarse table was generated with 50 grid points uniformly distributed between zero and 1500 V/cm for the electric field using a collision number of $10^8$. The Monte Carlo tracking of electrons using this coarse table was only used in the parallel plate example (shown in Appendix C) and to examine the parallelization scheme. The effects of these parameters on the induced current need further investigation.

The MPFD was evaluated using the more-accurate microscopic algorithm, which is directly based on the electron scattering cross sections with the gas atom in the Magboltz
database. Hence, a gas table is not necessary for the microscopic algorithm. Because the statistics error introduced in generating the table is avoided, the microscopic treatment is more accurate than the Monte Carlo integration algorithm.

### 7.5.2 Component Classes

In the component classes, the geometry is defined, the initialized MediumMagboltz gas is used to fill the geometry, and the electric field inside the gas volume is specified, i.e., the model is described. The constant, analytic, and field map component classes are provided. The constant component class defines a constant electric field. The analytic component class calculates simple electric fields created by two-dimensional wires, planes, or tubes using the capacitance matrix method. In these two component classes, the geometry must be defined in Garfield++ by using the basic GeometrySimple or the more advanced GeometryRoot classes.

For more complicated electric fields, the field map component classes are provided to read the electric field computed by other means (e.g., Elmer), which are summarized in Table 7.1. When the field-map files are imported into Garfield++ via the field map component class, the geometry defined in the third-party software is also constructed. Therefore, it is not necessary to define the geometry. In this work, the ComponentElmer class was used to read the result files generated by Elmer. The defined argon gas was used to fill the gas volume, i.e., body 1 in Elmer.

<table>
<thead>
<tr>
<th>Software</th>
<th>Component class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ansys</td>
<td>ComponentAnys121 for 2-D geometry</td>
</tr>
<tr>
<td></td>
<td>ComponentAnys123 for 3-D geometry</td>
</tr>
<tr>
<td>Synopsys TCAD</td>
<td>ComponentTcad2d for 2-D geometry</td>
</tr>
<tr>
<td></td>
<td>ComponentTcad3d for 3-D geometry</td>
</tr>
<tr>
<td>Elmer</td>
<td>ComponentElmer</td>
</tr>
<tr>
<td>CST</td>
<td>ComponentCST</td>
</tr>
<tr>
<td>COMSOL</td>
<td>ComponentComsol</td>
</tr>
</tbody>
</table>

Table 7.1: Field map component classes to read results from different softwares.
Mesh Quality

Garfield++ includes a built-in capability to check the imported finite element quality. When an electron is tracked in the gas, the finite element that contains the electron position is searched using the FindElement13 function to calculate the electric field. If the quality of the located finite element does not meet the criteria, the user is altered. Then, the electron that resides in the tracking geometry is killed due to the poor-quality element, which introduces error. Hence, a field map with sufficient quality is necessary for correct simulation. It was tested that in the Gmsh meshing of MPFD geometry, defining elementary points with characteristic length of 0.02 and turning on the CharacteristicLengthFromCurvature option can generate finite elements with sufficient quality.

Accelerating Finite Element Searching

Although the settings and options described above had led to electric field maps with high quality, the number of elements in the map was large (and, hence, computations became excessively costly). Because the original searching algorithm in the FindElement13 function is not efficient, it was time-consuming to locate the element. In the default searching algorithm, at a new electron position, it is first checked whether the new position is in the caching box of last element. If not, a search from the first element in the map is performed, and at each iteration, the caching box of the new element is computed. Hence, with large number of elements, which is required for sufficient mesh quality, looping over all the elements is computationally expensive.

To improve the performance, the optimized search techniques were used [81]. In the optimized algorithm, the caching box of each element is calculated before the simulation. If an electron leaves the old element, the neighbor elements are first checked instead of searching from the first element. In addition, the tetrahedral tree structure is used. These techniques have been implemented in the Garfield++ source code; however, they are not documented in the user guide [82]. The new search algorithm was enabled using the EnableTetrahedralTreeForElementSearch function in the ComponentElmer class.
7.5.3 Track Classes

Garfield++ provides two classes for simulating the energy loss of charge particle in gas, namely the TrackHeed and the TrackSrim classes. The TrackHeed class uses the HEED program [83] to simulate the ionization of charged particles with relativistic energy using the photo-absorption ionization model, i.e., the energy loss is minimal compared to the initial kinetic energy. This class is mainly used to simulate detectors for high-energy physics experiments.

The TrackSrim class was used in this work. This class reads a SRIM-generated table that describes the energy loss of ions in a gas to simulate the ionization of fission fragment. The SRIM tables of $^{95}_{38}$Sr and $^{139}_{54}$Xe in argon gas were calculated. This representative fission fragment pair was selected because of the high fission yield of about 0.05 [84], i.e., at the peak of the $^{235}$U fission fragment distribution. Because argon gas has a density of $1.784 \times 10^{-3}$ g/cm$^3$ at 0 °C and one atm, at 50 °C and 30 psig, according to the ideal gas law, the density was set to $4.586 \times 10^{-3}$ g/cm$^3$ in the SRIM-generated tables.

The SRIM tables were imported into Garfield++ using the TrackSrim class. In this class, the work function and Fano factor of argon gas were set to 27 and 0.19 eV, respectively [44]. The atomic and mass numbers of Ar were set to 18 and 40, respectively. The initial kinetic energies of $^{95}_{38}$Sr and $^{139}_{54}$Xe were set to 101.9 and 69.8 MeV, respectively [23]. One thousand $^{95}_{38}$Sr and one thousand $^{139}_{54}$Xe ions were simulated. It should be noted that it is an approximation to simulate one representative fission pair, and in the future work, a more comprehensive fission fragment distribution needs to be studied. The fission fragments were born uniformly in the fissile layer (shown in Fig. 7.1) at time zero with directions sampled isotropically into the gas-facing half space.

The TrackSrim class simulates the ionization of a fission fragment in the gas and creates electron clusters along its path, where a cluster is a group of electrons with same initial condition. In the calculations, along the track of a fission fragment, the maximum number of clusters was set to 5000 [85]. For each cluster, the ($x, y, z$) coordinate, the time of creation, the number of electrons (in the cluster), the energy deposited to create the cluster, and the
ion’s energy when the cluster was created can be retrieved using the `GetCluster` function. This cluster information is then used thereafter to initialize the electrons to be transported.

It was impractical (and probably not necessary) to transport all the electrons in the clusters to calculate the induced current, which requires that a compromise is made when considering the computing power available and the accuracy desired. In at least one past study, just a single electron per cluster was transported to calculate the signal with apparently sufficient accuracy [85]. In this study, the optimized element search techniques and the parallelized scheme (shown in the following) allowed tracking more electrons using the most-accurate (and time-consuming) microscopic tracking method for best accuracy. To evaluate the MPFD, 1% of the electrons in each cluster were transported to calculate a more-accurate shape of the induced current for future validation. According to the following MPFD results, one percent corresponded to about 10 to 30 electrons per cluster. The induced current by these 1% electrons was re-factored by 100 to represent the total signal. The systematic error introduced by not tracking all the electrons has not been formally quantified and needs further investigation.

**Fission Fragment Adjustment**

It was reported that grouping the electrons into clusters introduces a bias [85]. When the fission fragment collides with an atom of the gas, the fragment is deflected. Over the whole path of the fission fragment, this deviation, measured by the lateral straggling in the SRIM table, is relatively small compared to the range. However, grouping the electrons into clusters in Garfield++ over-estimates the deviation.

In the MPFD simulation, because the fission fragments were born in the fissile layer near the boundary of the gas volume, as a result of the over-estimated deviation, about 40% to 50% of the sampled fission fragments left the gas volume with only one or two clusters generated, which was a simulation artifact. To avoid this bias, sampling of the ionization of fission fragment in the gas was repeated until the number of clusters was larger than two. Thus, each of the two thousands simulated fission fragments ionized more than two clusters
of electrons. It has been shown that with such a correction, the Garfield++ simulated results still follow the range and straggling provided by SRIM [85], i.e., the fission fragment adjustment does not introduce an extra bias.

Cluster Time Adjustment

Garfield++ neglects the time that a fission fragment takes to pass through the gas volume, and for fission fragments that enter the gas volume at time zero, all the electron clusters are created at time zero. For best accuracy, the cluster-creation time was adjusted taking into consideration the flight time of the fission fragment [85].

Specifically, the first cluster was created at time zero. Each of the following clusters was created at time

\[ t_i = \frac{||\vec{P}_i - \vec{P}_{i-1}||}{v_i} + t_{i-1}, \]  

(7.1)

where \( \vec{P}_i \) and \( \vec{P}_{i-1} \) were the coordinates of the \( i \)th and the \((i - 1)\)th clusters, respectively, and \( t_{i-1} \) was the creation time of the \((i - 1)\)th cluster. The velocity of the fission fragment \( v_i \) was calculated by

\[ v_i = \sqrt{\frac{2E_a}{m}} \]  

(7.2)

\[ E_a = \frac{(E_{i-1} - dE_{i-1} + E_i)}{2}. \]

\( m \) was the mass of the fission fragment. \( E_a \) was the average kinetic energy of the fission fragment during the flight. After the \((i - 1)\)th cluster was created, i.e., the start point of the flight, the energy of the fission fragment was \( E_{i-1} - dE_{i-1} \), where \( E_{i-1} \) was the kinetic energy of the fission fragment when the \((i - 1)\)th cluster was created, and \( dE_{i-1} \) was the energy spent to create the \((i - 1)\)th cluster. \( E_i \) was the energy of the fission fragment when the \( i \)th cluster was created, i.e., the end point of the flight. These variables to calculate the adjusted cluster-born time were provided by the GetCluster function in the TrackSrim class.
7.5.4 Electron Transport Classes

Garfield++ provides three different algorithms of increasing fidelity for tracking charge carriers in the gas: Runge-Kutta-Fehlberg (RKF) integration, Monte Carlo integration (class name \texttt{AvalancheMC}), and a microscopic tracking technique (class name \texttt{AvalancheMicroscopic}). While the avalanche physics is implemented in the last two methods, it is not of importance in MPFDs. All the three methods can not simulate the electron recombination physics [85]. The last two methods were used in this study to transport electrons.

Monte Carlo Integration

The Monte Carlo integration method can be used to track electrons or ions in gas using a table that contains the transport properties of the charge carrier. For electrons in gas, this table can be computed by the built-in interface to the Magboltz program, as discussed in Section 7.5.1, to provide the electron transport properties in most common gas mixtures. Based on the electron transport properties, the Monte Carlo integration method simulates the drift under electric field, diffusion, attachment, and Townsend processes. In addition, the \texttt{AvalancheMC} class has the \texttt{DisableDiffusion} function to exclude the simulation of the diffusion process, which may be used to analyze the effects of diffusion on the induced current.

The ion transport table can not be directly calculated in Garfield++. In the Garfield++ source code (version v1r0), ion tables for argon, carbon dioxide, helium, and neon gases at temperature 300 K are provided. While unneeded in this study, transport of other ions is possible by providing the necessary table.

In a Monte Carlo step, a drift length $\Delta s = v_d \Delta t$ is computed. A $\Delta t$ of 0.01 ns was used in this study. The drift speed $v_d$ at local electric field is calculated using Eq. (2.4). Then, a random diffusion step is sampled from three uncorrelated, Gaussian distributions with standard deviation $\sigma_L = D_L \sqrt{|\Delta s|}$ for the component parallel to $v_d$ and standard deviation $\sigma_T = D_T \sqrt{|\Delta s|}$ for the two transverse components. $D_L$ and $D_T$ are the corresponding diffusion coefficients. The drift and diffuse steps are added to construct the traveling length. The
simulation of the diffusion process can be turned off using the DisableDiffusion function, which may be useful to analyze its effects on the induced current.

In a Monte Carlo step, a drift length $\Delta s = v_d \Delta t$ is computed. A $\Delta t$ of 0.01 ns was used in this study. The drift speed $v_d$ at local electric field is calculated using Eq. (2.4). Then, a random diffusion step is sampled from three uncorrelated Gaussian distributions with standard deviation $\sigma_L = D_L \sqrt{|\Delta s|}$ for the component parallel to $v_d$ and standard deviation $\sigma_T = D_T \sqrt{|\Delta s|}$ for the two transverse components. $D_L$ and $D_T$ are the corresponding diffusion coefficients. The drift and diffuse steps are added to construct the traveling length. The simulation of the diffusion process can be turned off using the DisableDiffusion function, which may be useful to analyze its effects on the induced current.

In this work, the Monte Carlo integration method was only used in the parallel plate example shown in Appendix C and to examine the parallelization scheme based on a coarse electron transport table.

**Microscopic Tracking**

The microscopic method can only track electrons. This method simulates the electron transport in gas using the Monte Carlo method based on the electron-molecule scattering cross sections provided by the Magboltz program. Hence, the electron transport table as used in the Monte Carlo integration method is not necessary. The statistical error introduced by use of the pre-generated table is avoided in the microscopic tracking method, which makes it more accurate than the Monte Carlo integration method.

The detailed physics of the microscopic tracking method is not specified in the Garfield++ user guide [82]. From the source code, the algorithm implemented by this method is like the Monte Carlo flow to transport neutrons, as stated in Section 3.2. Specifically, based on the cross section, the collision type of a colliding electron is sampled to be elastic, ionization, attachment, inelastic, excitation, super-elastic, one of several possible phonon-related scatterings, or coulomb scattering. The electron condition after a collision is sampled accordingly. Therefore, more interactions are simulated in the microscopic tracking method,
which is another contribution that makes it more accurate than the Monte Carlo integration method. The microscopic method was used to evaluate the MPFD.

### 7.5.5 Parallelization Scheme

A fission fragment deposits a few MeV energy in the gas volume of MPFD, which creates about $10^5$-$10^6$ electron/ion pairs grouped into clusters. To track 1% of these electrons using the time-consuming microscopic tracking method is beyond the capability of the serial Garfield++ code. Hence, an application parallelized by hybrid Message Passing Interface (MPI) and OpenMP was developed. The pseudo-code of the parallelization scheme is shown in Algorithm 1. Two thousand fission fragments were distributed among the computing nodes using MPI. On each node, the transport of the 1% ionized electrons was simulated by the cores using OpenMP. Each computing node was initialized with its own random seed automatically by the underlying ROOT program.

In the code, after the MPI initialization, a set of MediumMagboltz, ComponentElmer, Sensor, and TrackSrim class objects is initialized. These utilities are owned by one core on the node and used to simulate the ionization of the fission fragments. The MediumMagboltz object defines the argon gas at 30 psig and 50 °C. The ComponentElmer object imports the field map computed by the Elmer program and assigns the defined MediumMagboltz object to fill the gas volume, i.e., body 1 defined in ElmerSolver. In addition, the ComponentElmer objects enables the optimized element searching algorithm. The MediumMagboltz and the ComponentElmer objects define the material and geometry and complete the model description. The ComponentElmer object is linked to a Sensor instance, which connects the model to the TrackSrim class instances. Two TrackSrim instances are initialized reading the SRIM energy loss tables of Sr and Xe, respectively.

The ncluster and nsignal C++ vectors are used to store the computed cluster information and induced current by the assigned fission fragments on the node, respectively.

Another set of thread-private class objects is initialized inside an OpenMP parallel construct to transport the electrons via the AvalancheMicroscopic class object. This set is
Algorithm 1 Pseudo-code of the Garfield++ parallelization scheme.

1: Initialize MPI
2: Initialize MediumMagboltz, ComponentElmer, Sensor, and TrackSrim class objects
3: Initialize ncluster, nsignal –– vectors to store cluster and signal on the node
4: #pragma omp parallel
5: Initialize thread-private MediumMagboltz, ComponentElmer, Sensor, and AvalancheMicroscopic class objects
6: end omp parallel
7: for ff ← [0, 2000) do
8:   if ff % number of nodes == rank then –– assign ff to MPI rank
9:     Initialize fcluster, fsignal –– vectors to store ff cluster and signal
10:   Determine ff is Sr or Xe
11:     while true do –– track ff to create electron clusters
12:       fcluster → clear
13:       Sample position and direction of ff
14:       TrackSrim → NewTrack(position, direction)
15:       fcluster ← (TrackSrim → GetCluster)
16:       if fcluster.size > 2 then
17:         break
18:     end if
19:   end while
20: Adjust cluster time considering flight of fission fragment
21: Initialize cmap –– construct cluster map for 1% electrons
22: #pragma omp parallel
23: iSensor → ClearSignal –– isensor: thread-private Sensor objects
24: #pragma omp for
25:   for i ← [0, cmap.size) do
26:     AvalancheMicroscopic → AvalancheElectron(cmap[i])
27:   end for
28: #pragma omp critical
29:   fsignal += isignal → GetSignal
30: end omp critical
31: end omp parallel
32: Append fcluster to ncluster
33: Append fsignal to nsignal
34: end if
35: end for
36: Print ncluster, nsignal×100
37: Finalize MPI

static and exists until the simulation ends. Therefore, this utility set only needs to be initial-
ized for once. Each core has the same utility set between two OpenMP parallel constructs,
e.g., between the simulation of two successive fission fragments. The AvalancheMicroscopic
object links to the Sensor object to reads the material and geometry. In addition, the calculated induced current by the AvalancheMicroscopic object is also retrieved via the Sensor instance. The induced current between time zero and 1 µs was calculated with a time bin of 0.01 ns.

Simulation of the two thousand fission fragment histories is distributed among the MPI ranks, i.e., computing nodes. Half of the histories are $^{95}_{38}$Sr, and the other are $^{139}_{54}$Xe. Inside the loop, the fcluster and the fsignal C++ vectors are initialized to store the cluster information and induced current of this fission fragment. The fission fragment is sampled to be born uniformly in the fissile layer with an isotropic direction towards the gas volume. The TrackSrim object is used to track the fission fragment with the sampled position and direction. The process is repeated until the number of electron clusters created by the fission fragment is larger than two, as stated in Section 7.5.3. The sampled cluster information is stored in the fcluster vector. Then, the cluster time is adjusted according to the method presented in Section 7.5.3. A cmap C++ vector is initialized to store the cluster identification numbers of those 1% of electrons tracked.

A team of cores on the node is formed in an OpenMP parallel construct to simulate the transport of electrons. The signal stored in the thread-private Sensor object is first cleared. Transport of the electrons is distributed to the cores using the OpenMP loop construct. The initial condition of the electron is read from the cmap vector using the cluster identification number, e.g., the $xyz$ coordinates and the birth time. The electrons are assumed to begin with zero initial energy and random directions.

The electrons are transported using the AvalancheElectron function defined in the AvalancheMicroscopic class. When the transport of the electrons is finished, the induced current in each core is accumulated to the fsignal vector in an OpenMP critical construct to compute the induced current of this fission fragment. Then, the fcluster and the fsignal vectors are appended to the ncluster and the nsignal vectors, respectively. When a node finishes the simulation of the assigned fission fragments, it prints out the cluster information and signal (re-factored by 100) of each fission fragment for post processing.

To examine the correctness of the parallelization scheme, a particular MPFD calculation
was performed using one core and 10 ten-core nodes. In this calculation, 500 fission fragments were simulated, half of which were Sr ions, while the remainder were Xe ions. The Monte Carlo integration method was used to track 0.5% of the electrons in each cluster. The diffusion process was not simulated.

The computed induced currents of the two runs are shown in Fig. 7.7. The small difference may be explained by the facts that 1) the systematic error introduced by tracking only 0.5% electrons per cluster was not included; 2) the 500 fission fragments were born uniformly in the fissile layer and had isotropic directions, and 3) electron clusters were created with statistics. In the future work, a rigid comparison is warranted that the same set of random numbers was used by the serial and parallel runs to examine whether the two results are identical.

![Figure 7.7: The computed induced current using one and 10 x 10 cores.](image)

7.6 MPFD Results

Two thousand fission fragments were simulated using the microscopic tracking method. The averaged deposited energy per fission fragment to create electron clusters was $7.15 \pm$
0.14 MeV. Along the path of a fission fragment, on average, 118.41 ± 2.34 electron clusters were created. The average number of electrons created by a fission fragment was $2.65 \times 10^5 \pm 5.12 \times 10^3$.

Shown in Fig. 7.8 are the induced currents by three fission fragments, and shown in Fig. 7.9 is the average induced current of the two thousand fission fragments. A peak exists at about 0.3 ns, which may be due to the diffusion of the electrons born near the boundary.

![Figure 7.8: Induced currents by three fission fragments.](image)

For each fission fragment, the collected charge $Q$ by the induced current $i$ can be calculated by

$$Q = \int_0^{t_e} i(t) dt,$$

where $t_e$ is the end time of the integration. In practice, $t_e$ represents an ideal $RC$ circuit setting in the experimental measurement to truncate the signal after the majority of the electrons are collected. If $t_e$ was set to the maximum of the tally window, i.e., 1 $\mu$s, the total charge can be computed. It is shown in Fig. 7.8 and Fig. 7.9 that 1 $\mu$s is sufficient to collect the electrons in the MPFD. Then, the time necessary to collect 95% of the total charge can be located. The total charge and the time to collect 95% of the total charge of
the two thousand fission fragments are shown in Fig. 7.10. 57% of the fission fragments can generate total charges larger than 2 fC, and 98.5% of the two thousand ionization events need less than 400 ns to collect 95% of the total charge. The collected charges are in the fC scale, and, hence, the signal from the MPFD needs to be amplified in the external circuit to be measured.

Shown in Fig. 7.11 is the distribution of the time to collect 95% of the total charge of the two thousands fission fragments. The majority of the induced currents are within 400 ns.

The distribution of the deposited energy by the fission fragments to create electron clusters is shown in Fig. 7.12, and the distributions of the collected charges integrated to 400 ns and 1 µs are shown in Fig. 7.13. The shapes of the two charge distributions agree well, i.e., an integration time of 400 ns is sufficient to collect the majority of the electrons. The charge distributions reveal the shape of the deposited energy distribution, because the electron recombination was not simulated. The integration time of 400 ns is sufficient to collect the majority of the electrons.
Figure 7.10: Correlated total charge and time to collect 95% of the charge.

Figure 7.11: Distribution of the time to collect 95% of the total charge.

7.7 Summary

A computational tool to evaluate the electron collection process in MPFDs was developed. Gmsh and Elmer were used to calculate the electric field map in the gas volume of MPFD
Figure 7.12: Distribution of the deposited energy to create electron clusters.

Figure 7.13: Distribution of the collected charge.

using the finite-element method. The energy losses of the representative Sr and Xe fission fragment pair were calculated by SRIM. With the Elmer and SRIM outputs, Garfield++ was used to simulate the ionization of fission fragments, transportation of electrons, and compu-
tation the induced current. In particular, the built-in optimized element search techniques and the developed parallelization scheme by hybrid MPI and OpenMP allowed simulation of 1% of the ionized electrons per cluster by the fission fragments using the most-accurate microscopic tracking method. According to the results, the fission fragments deposited an average of 7.15 MeV energy in the gas by ionizing electrons, which were collected within 400 ns. The results suggest that the MPFD as designed can provide a fast response for in-core applications. Indeed, the results presented are preliminary, and the merit of this chapter is to explore a promising method to model the MPFD. As part of future work, the computational tool should be verified and validated to assist the development of the MPFD technology and to understand its response from the initial signal creation through the electronics system.
The restart of the TREAT facility brought back the transient test capability for nuclear fuels and materials to U.S.. After the restart, the facility will be first used to test the accident tolerant fuels used in contemporary nuclear reactor cores to improve safety. While the facility has been restarted, alternative neutron-detection techniques used in the hodoscope and in the TREAT core are under development at Kansas State University. In this work, the ZnS(Ag) scintillation detectors and fast-sensitive MSNDs for the hodoscope, and the MPFDs to measure in-core neutrons were evaluated using different computational tools to simulate the underlying physics. The calculations span the simulation of scintillation, semiconductor, and gas-filled detectors, which are the three common categories of neutron detectors.

The ZnS(Ag) scintillation detectors were modeled using Geant4 to simulate the coupled nuclear and optical physics. The Hornyak button fast-neutron detector used in the original TREAT hodoscope was first evaluated to validate the computational methodology and physics models. Under a hodoscope-like radiation environment, a neutron-detection efficiency of 0.35% was predicted at an S/N ratio of 100 consideration the scintillation noise.
generated by gamma rays. The efficiency agrees relatively well with the reported experimental value of 0.4%, where the pulse-shape discrimination was applied. The strong gamma-induced Cherenkov noise was also observed in the simulation.

8.1.2 Hornyak Button Variants

To reduce the gamma-induced Cherenkov noise and to improve the neutron-detection efficiency, the layered and the homogenized Hornyak button variants were proposed. The new detectors use SiPMs to collect light, which is more efficient and reduces the Cherenkov noise generated in the combination of Lucite light guides and the PMT used in the Hornyak button. The improved light-collection method allows a higher concentration of ZnS(Ag) in the scintillation volumes of the new detectors to increase the neutron-detection efficiency.

Using the same methodology to evaluate the Hornyak button, it was predicted that the Cherenkov noises in the new detectors were reduced. To reject the gamma-induced scintillation and Cherenkov noises using the pulse-height discrimination, at the LLD settings that achieved an S/N ratio of 100, the optimized, 5-cm layered and homogenized detectors yielded neutron-detection efficiencies of 3.3% and 1.3%, respectively. By increasing the detector length along the mono-direction neutron path, the neutron-detection efficiencies were shown to saturate at about 5.9% and 2.2% for the layered and the homogenized devices, respectively. For more intense gamma-ray background (gamma-to-neutron ratios above 50), the homogenized detector exhibited better performance than the layered detector due to the less insensitivity of the homogenized scintillation volume to the incident gamma rays.

8.1.3 Fast-Sensitive MSNDs

The fast-sensitive MSNDs use fast-neutron converters to replace $^6$LiF loaded in the well-established thermal-sensitive devices. The neutron converters considered were $^{237}$Np, $^{235}$U, natural uranium, and $^{232}$Th for actinide MSNDs and paraffin wax for hydrogenous MSNDs. Paraffin wax has a larger fission-spectrum-weighted macroscopic cross section (0.32 cm$^{-1}$) than the actinide materials (the best being 0.067 cm$^{-1}$ for $^{237}$Np). However, the actinide
reactants allow higher LLD settings due to the large energy of fission fragments.

Using the fission fragment generator in Geant4 to evaluate the actinide MSNDs, at the 5-MeV LLD setting, the intrinsic neutron-detection efficiency of the $^{235}$U-filled MSND was 1.2% for a 2-cm device length, and the efficiency saturated at 2.6% for lengths beyond 14 cm. The trench and wall widths in the $^{235}$U-filled MSNDs were 20 and 10 µm, respectively, which is the current configuration of thermal-sensitive devices. For the 2-cm $^{235}$U-filled MSND, the Geant4-computed, total deposited energy in the trenches differed from the MCNP6-predicted value by about 0.7%. The efficiencies of the $^{235}$U-filled MSNDs acted as the lower limits of the $^{237}$Np-loaded devices, which are preferred due to their insensitivity to the slow neutrons. The $^{237}$Np-filled MSNDs were not evaluated in Geant4 due to the absence of neutron data library.

Geant4 and MCNP6 were used to calculate the neutron event pulse height distributions of the hydrogenous MSNDs, and the results of the two codes agreed well. At 300-keV LLD setting, the intrinsic neutron-detection efficiencies of the hydrogenous MSNDs were 10% and 26% at the device lengths of 2 and 20 cm, respectively, where the 20-µm trench and 10-µm wall widths were assumed.

Geant4 was used to compute the pulse height distributions of the hydrogenous MSNDs irradiated by the hodoscope-like gamma rays. Based on the predicted gamma noises, at the LLD settings that achieve an S/N ratio of 100, the neutron-detection efficiencies were about 2.5% and 9.6% for the hydrogenous MSNDs with device lengths of 2 and 20 cm, respectively, where the optimized 60-µm trench and 40-µm wall widths were applied.

### 8.1.4 MPFD

To evaluate the electron-collection process under applied electric field in MPFD, a computational routine that consists of Gmsh, Elmer, SRIM, and Garfield++ was developed. The electric field in the MPFD gas volume was calculated by Gmsh and Elmer using a finite-element method. The energy loss tables of the representative Sr and Xe fission fragment pair were computed by SRIM. With the Elmer and SRIM results, Garfield++ was used to simu-
late the ionization of fission fragments, transport of electrons in the argon gas, and calculate the induced current as a function of time. In particular, the built-in, optimized element search techniques and the developed hybrid MPI and OpenMP parallelization scheme were used to build the Garfield++ application, which allowed the simulation of 1% electrons ionized by 2000 fission fragments using the microscopic tracking algorithm. In the simulation, 100-V voltage was applied to the anode, and the cathode was grounded. The temperature and pressure of the argon gas inside the MPFD were 50 °C and 30 psig, respectively. Under such condition, the averaged deposited energy to ionize electrons was about 7.15 MeV, and for the majority of the simulated neutron events, the induced current occurred within 400 ns.

### 8.2 Future Work

#### 8.2.1 Testing of the Hodoscope Detectors

While the modeling results of the hodoscope detectors are promising, they need to be tested to validate the computational results. Ideally, the detectors need to be tested in the hodoscope which is not currently available. As a compromise, the piercing beam at the Kansas State University TRIGA Mark II reactor can be used to test the detectors. However, the beam is not fully characterized and known to be dominated by sub-fast neutrons and gamma rays. Ongoing efforts are to design appropriate filters used at the beam port to mimic the hodoscope radiation environment [86]. Upon completion of this characterization the construction of suitable filters, the beam can be a good facility to test the fast-neutron devices, and the detector performance under the characterized beam radiation can be calculated using the existing models.

As a first demonstration, the prototypes of the layered Hornyak button variants were fabricated and irradiated using a $^{252}$Cf source, and a neutron-detection efficiency of 9.2% was observed for a device length of 4 cm [87, 88].
8.2.2 Expanding the MPFD Modeling

Due to the time consideration, the MPFD modeling results are preliminary, and the methodology can be considered explored and neither verified completely nor validated yet against experimental data. It is not convenient to navigate the underlying codes to make any changes because each code has its own syntax. Hence, a governing application should be developed that integrates the underlying codes and gives access to set the input parameters easily.

A rigid verification of the parallelization scheme is necessary, where the same set of random numbers are used by the serial and parallel runs. The scaling performance of the parallelization scheme needs to be evaluated.

The modeling results of MPFD were calculated using the most-accurate microscopic tracking method. In the future work, the Monte Carlo integration method needs to be explored, in which the simulation of the diffusion process can be turned off. This feature can be used to evaluate the effects of the diffusion process on the induced current.

It is difficult to compare the calculated MPFD results against in-core measurements considering the complexity of in-core radiation environment. Therefore, an out-of-core MPFD prototype might be necessary for the validation purpose.
Bibliography


Appendix A

MCNP and Geant4 Inputs

An example problem was modeled in MCNP and Geant4 to compare the inputs. The details of the problem are shown in Fig. A.1. The global volume is a cube with 20-cm length filled with dry air. At the center of the global volume is a cubic tank filled with paraffin wax. The tank has 10-cm length and spans from -5 to 5 cm in the $xyz$ axes. A point source is located at $(-6, 0, 0)$ cm, i.e., 1-cm away from the tank, and shoots neutrons with 1-MeV energy into the tank along the $x$ axis. The tally is the total deposited energy in the tank. The problem was modeled in Geant4 10.3.1 and MCNP6.1.

Figure A.1: An example problem was modeled in Geant4 and MCNP to compare the inputs. All dimensions are in cm.
A.1 MCNP Input

The MCNP input is shown in Fig. A.2, which consists of cell, surface, and several data cards.

A.1.1 Surface Cards

In the surface cards, surface 1 is a rectangular parallelepiped macrobody (with keyword rpp), which spans from -10 to 10 cm in the $xyz$ axes. Surface 1 is used to describe the global volume. Surface 2 is defined in the same way as surface 1, and surface 2 is used to model the tank filled with paraffin wax.

A.1.2 Cell Cards

A cell card consists of the cell number, filled material, and bounding surfaces to describe the volume. Specially, cell 1 is void (indicated by 0) and defines the volume outside surface 1. The volume outside a macrobody is positive with respect to the surface number. Cell 2 is filled with material 1 (dry air) with density of 0.001205 g/cm$^3$. The negative density value indicates the unit of g/cm$^3$. The cell is inside surface 1 and outside surface 2. Cell 3 is filled with material 2 (paraffin wax) with density of 0.93 g/cm$^3$, and it is inside surface 2.

A.1.3 Data Cards

Material Cards

A material card consists of material number, nuclide identifiers and corresponding fractions. A nuclide identifier is formed by the $ZA$ number and the data table identification number. The fraction can be specified by mass fraction using negative value or by atom fraction as positive.

Material 1 defines the dry air and consists of natural abundance carbon (6000), $^{14}\text{N}$ (7014), $^{16}\text{O}$ (8016), and natural abundance argon (18000), and the mass fraction of these nuclides are specified. In the data table identification number, 70 represents the Endf70a library at 293.6 K, and c stands for continuous-energy neutron tables. The Endf70a library
A simple MCNP example

```plaintext

A simple MCNP example

c cell card
1 0 1 $ outside world
2 1 -0.001205 -1 2 $ air surrounding tank
3 2 -0.93 -2 $ in tank

c surface card
1 rpp -10 10 -10 10 -10 10 $ world
2 rpp -5 5 -5 5 -5 5 $ tank

c data card

c material cards

c dry air, rho = 0.001205
m1 6000.70c -0.000124 &
  7014.70c -0.755268 &
  8016.70c -0.231781 &
  18000.59c -0.012827

c paraffin wax, C25H52, density = 0.93 g/cm3
m2 1001.70c 52 &
  6000.70c 25

c importance cards
imp:n 0 1 1
imp:h 0 1 1
imp:p 0 1 1
imp:# 0 1 1
imp:e 0 1 1

c mode card
mode p h # n e

c cut off card
cut:h j 0 $ default = 1 MeV
cut:# j 0 $ default = 5 MeV

c neutron physics
phys:n 6j 4

c tally card
+f6 3
sd6 1

c source card
sdef par=n erg=1 x=-6 y=0 z=0 vec=1 0 0 dir=1
nps 1000
print 110

Figure A.2: MCNP input of the simple model.
```
for natural abundance argon (18000) is not available, and, thus, the Misc5xs library (with identification number 59) at 293.6 K is used. The available data libraries are listed at Appendix G, Volume I of the MCNP5 manual [62]. Material 2 defines the paraffin wax (C_{25}H_{52}) using atom fractions.

**Importance and Mode Cards**

In the mode card, neutron (n), proton (h), photon (p), ion (#), and electron (e) are tracked for best accuracy. The importances for these particles in cell 1 to 3 are zero, one, and one, respectively.

**Cutoff Cards**

The default low kinetic-energy cutoffs for proton and ion are 1 and 5 MeV, respectively, which are too high for this problem. Hence, the cutoffs are lowered to zero for best accuracy. In practice, MCNP6 adjusts these zero cutoffs to the minimum value of 1 keV. The default cutoffs for neutron (0), photon (1 keV), and electron (1 keV) are used and not specified.

**Neutron Physics Card**

The first 6 input parameters in the neutron physics card are skips by the 6j shortcut. The 7th parameter, coilf, is set to 4, which generates one ion from neutron elastic scattering and uses the neutron capture ion algorithm (NCIA) to sample the capture reaction with ^3He, ^6Li and ^10B (though these nuclides are not present in this problem). The NCIA preserves the correlation of the secondary particles, e.g., ^3H and ^4He in the ^6Li reaction. This coilf value is recommended in the MCNP6 manual [35].

**Tally Cards**

The +f6 collision heating tally is used to compute the deposited energy in cell 3. In default, this tally applies to all tracked particles, and, thus, no particle designator is needed. The unit of +f6 tally is MeV/g. For convenience, the mass of the tally cell 3 is set to 1 g using the
segment divisor (sd) card. Then, the magnitude of the +f6 tally gives the history-averaged deposited energy in MeV.

Source Card

Neutrons (par=n) with 1-MeV energy (erg=1) are born at position (−6, 0, 0) cm and travel along the x axis, i.e., the cosine value with respect to the reference vector (1, 0, 0) is one (dir=1). One thousand such neutrons are simulated (nps 1000), and table 110 is printed to verify the source sampling.

The computed deposited energy in paraffin wax is 0.917 ± 1.94%, or between 0.899 to 0.935, MeV per source neutron.

A.2 Geant4 Input

A.2.1 Main Function

Inputs of the Geant4 application for the example problem consist of customized C++ classes coordinated by a main function, which is shown in Listing A.1. In the included headers, globals.hh contains the Geant4-derived basic data types, e.g., G4double and G4int, to replace the standard C++ counterparts, e.g., double and int, which ensures value-range consistency for different compilers and platforms. G4SystemOfUnits defines the units.

In the function body, an instance of the G4MTRunManager class is initialized, which is used in a multi-thread run. The number of cores to run the simulation is set to the available cores on the node. Instances of the DetectorConstruction, ActionInitialization, and QGSP BERT HP reference physics list classes are registered to run manager. The singleton object of the G4UImanager class reads the macro commands from the command-line file. In the end, the memory of the run manager class instance is freed, which implicitly deletes the registered class objects.
Listing A.1: main.cc

```cpp
#include "globals.hh"
#include "G4SystemOfUnits.hh"
#include "G4MTRunManager.hh"
#include "DetectorConstruction.hh"
#include "QGSP_BERT_HP.hh"
#include "ActionInitialization.hh"
#include "G4UImanager.hh"

int main(int argc, char** argv)
{
    // initialize multi-thread run manager
    G4MTRunManager* runManager = new G4MTRunManager();
    runManager -> SetNumberOfThreads(G4Threading::G4GetNumberOfCores());
    // register detector construction, physics list, and action
    // initialization
    runManager -> SetUserInitialization(new DetectorConstruction());
    runManager -> SetUserInitialization(new QGSP_BERT_HP());
    runManager -> SetUserInitialization(new ActionInitialization());
    // UI manager
    G4UImanager* UImanager = G4UImanager::GetUIpointer();
    // batch mode + macro file
    G4String command = "/control/execute ";
    G4String fileName = argv[1];
    UImanager -> ApplyCommand(command + fileName);
    // run manager frees the memory for the registered classes
    if (runManager)
        delete runManager;
    return 0;}
```

A.2.2 Detector Construction

The DetectorConstruction class is defined in Listing A.2 and Listing A.3. This class inherits the Construct function from the G4VUserDetectorConstruction base class to pass the defined materials and geometry of the model into Geant4 kernel. Dry air and paraffin wax have been predefined in the internal material database, G4NistManager.

The world and the paraffin tank are defined in the same way. A Geant4 box solid is first defined with four parameters, which are name and half lengths in $xyz$ axes. The solid is
filled with material to construct the logical volume. The logical volume is placed into the tracking geometry via the physical volume, definition of which contains rotation matrix and translation vector with respect to the mother logical volume. No rotation and coordinate translation is needed for this model. The world physical volume has no mother volume, and, thus, a null pointer is entered. The world physical volume is returned to complete the construct.

Listing A.2: DetectorConstruction.hh

```cpp
#ifndef DetectorConstruction_h
#define DetectorConstruction_h

#include "globals.hh"
#include "G4SystemOfUnits.hh"
#include "G4VUserDetectorConstruction.hh"
#include "G4NistManager.hh"
#include "G4Material.hh"
#include "G4Box.hh"
#include "G4LogicalVolume.hh"
#include "G4PVPlacement.hh"

class DetectorConstruction : public G4VUserDetectorConstruction{
public:
    DetectorConstruction();
    virtual ~DetectorConstruction();
    G4VPhysicalVolume* Construct();
};

#endif
```

A.2.3 Action Initialization

Shown in Listing A.4 and Listing A.5 is the definition of the `ActionInitialization` class, which inherits the `G4VUserActionInitialization` class. In the `BuildForMaster` function, which is only called by the master thread, an instance of the self-developed `RunAction` class is initialized, which collects tallies from the local `RunAction` class objects. In the `Build` function, which is called by all the working threads, instances of the mandatory
Listing A.3: DetectorConstruction.cc

```cpp
#include "DetectorConstruction.hh"
DetectorConstruction::DetectorConstruction()
: G4VUserDetectorConstruction() {}  
DetectorConstruction:: ~ DetectorConstruction() {}  
G4VPhysicalVolume* DetectorConstruction:: Construct()  
{}  
// internal material database  
G4NistManager* nist = G4NistManager::Instance();  
G4Material* air = nist -> FindOrBuildMaterial("G4_AIR");  
G4Material* wax = nist -> FindOrBuildMaterial("G4_PARAFFIN");  
G4double len = 10.0 * cm;  
// cubic world solid, half lengths in xyz axes are specified  
G4Box* world_solid = new G4Box("world_solid", len, len, len);  
G4LogicalVolume* world_lv = new G4LogicalVolume(world_solid, air,  
"world_lv");   // logical volume consists of solid and material  
G4VPhysicalVolume* world_pv = new G4PVPlacement(  
0,  // rotation matrix  
G4ThreeVector(),  // translation vector  
world_lv,  // logical volume  
"world_pv",  // physical volume name  
0,  // mother logical volume  
false,  // future use  
0,  // copy number  
true);  // surface check  
// cubic tank solid, half lengths are specified  
G4Box* tank_solid = new G4Box("tank_box", len*0.5, len*0.5, len*0.5);  
G4LogicalVolume* tank_lv = new G4LogicalVolume(tank_solid,  
wax, "tank_lv");  
G4VPhysicalVolume* tank_pv = new G4PVPlacement(  
0,  // rotation matrix  
G4ThreeVector(),  // translation vector  
tank_lv,  // logical volume  
"tank_pv",  // physical volume name  
world_lv,  // mother logical volume  
false,  // future use  
0,  // copy number  
true);  // surface check  
return world_pv;;
```

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PrimaryGeneratorAction and three optional user action classes are initialized, which are RunAction, EventAction and SteppingAction. The PrimaryGeneratorAction class defines source particles. The user action classes are linked to accumulate tally, which was used in the neutron detector models. Other tally methods are also provided, e.g., multi-functional detector, primitive scorer, and command-based scoring [60].

Listing A.4: ActionInitialization.hh

```cpp
#ifndef ActionInitialization_h
#define ActionInitialization_h 1
#include "G4VUserActionInitialization.hh"
#include "PrimaryGeneratorAction.hh"
#include "RunAction.hh"
#include "EventAction.hh"
#include "SteppingAction.hh"

class ActionInitialization : public G4VUserActionInitialization
{
public:
    ActionInitialization();
    virtual ~ActionInitialization();
    virtual void BuildForMaster() const;
    virtual void Build() const;
};
#endif
```

Primary Generation

Shown in Listing A.6 and Listing A.7 is the PrimaryGeneratorAction class to define source particles via the G4GeneralParticleSource (GPS) class. The GPS class provides a relatively comprehensive macro commands to avoid hard coding.

The macro commands are listed in a macro file, as shown in Listing A.8. This macro file is read by the executable via command line, as indicated in Listing A.1.
Run Action

Shown in Listing A.9 and Listing A.10 is the customized RunAction class. The variables `rerg` and `rerg2` accumulate tally and tally square from events, respectively, to compute the
Listing A.7: PrimaryGeneratorAction.cc

```cpp
#include "PrimaryGeneratorAction.hh"

PrimaryGeneratorAction::PrimaryGeneratorAction()
    : G4VUserPrimaryGeneratorAction()
{ generator = new G4GeneralParticleSource(); }

PrimaryGeneratorAction::~PrimaryGeneratorAction()
{if (generator)
    delete generator; }

void PrimaryGeneratorAction::GeneratePrimaries(G4Event* anEvent)
{ generator -> GeneratePrimaryVertex(anEvent); }
```

Listing A.8: Macro file

```bash
# Initialize kernel
/run/initialize
# verbose setting
# control/verbose 0
/run/verbose 0
/event/verbose 0
/tracking/verbose 0
# GPS definition
# neutron
/gps/particle neutron
# position sampling
/gps/pos/centre -6 0 0 cm
# direction sampling
/gps/direction 1 0 0
/gps/ene/mono 1 MeV
/run/beamOn 1000
```

average and variance. The type of these variables instantiates the G4Accumulable template class using the G4double type, and, hence, the master instance of the run action class can merge tallies from local threads. The add_event_energy function is called at the end of each event to accumulate the event-specific tallies (shown in Listing A.12), and the cal_ave function computes the average and relative error. The computed results are printed at the end of the run by the master thread.
Event Action

The EventAction class is shown in Listing A.11 and Listing A.12. It has a data member, `event_erg`, to accumulate tally from steps via the `add_step_energy` function. At the beginning of an event, this variable is set to zero, and at the end of an event, non-zero event tally is accumulated via the `add_event_energy` function in the run action.

Step Action

Shown in Listing A.13 and Listing A.14 is the SteppingAction class. The UserSteppingAction function is called at the end of every Monte Carlo step to extract the tally. Each step has
# include "RunAction.hh"

RunAction::RunAction() : G4UserRunAction(), rerg(0.0), rerg2(0.0){
    // register accumulable
    auto accumulableManager = G4AccumulableManager::Instance();
    accumulableManager -> RegisterAccumulable(rerg);
    accumulableManager -> RegisterAccumulable(rerg2);
}

void RunAction::BeginOfRunAction(const G4Run* run) {}
void RunAction::EndOfRunAction(const G4Run* run) {
    // merge accumulables
    auto accumulableManager = G4AccumulableManager::Instance();
    accumulableManager -> Merge();
    // get value
    G4double verg = rerg.GetValue();
    G4double verg2 = rerg2.GetValue();
    // Print
    if (IsMaster()){  
        G4cout << "---------------- End of Global Run ------------------- \n";
        G4int nofEvents = run -> GetNumberOfEvent();
        vec_double ans = cal_ave(verg, verg2, nofEvents);
        G4cout << " Ave. total deposited energy in tank, relative error = " 

vec_double RunAction::cal_ave(G4double var, G4double var2, G4int n){
    vec_double ans(2);
    G4double ave = var / n, ave2 = var2 / n;
    ans[0] = ave;
    G4double std_dev = sqrt((ave2 - ave * ave) / (n - 1));
    if (fabs(ave) < 1.0e-20)
        // if no tally, set the relative error to 1
        ans[1] = 1.0;
    else
        ans[1] = std_dev / ave;
    return ans;}

void RunAction::add_event_energy(G4double eerg){
    rerg += eerg;
    rerg2 += eerg * eerg;}

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Listing A.11: EventAction.hh

```c++
#ifndef INCLUDE_EVENTACTION_HH_
#define INCLUDE_EVENTACTION_HH_
#include "G4UserEventAction.hh"
#include "globals.hh"
#include "RunAction.hh"

class EventAction : public G4UserEventAction
{
    public:
        EventAction(RunAction*);
        ~EventAction();
        void BeginOfEventAction(const G4Event*);
        void EndOfEventAction(const G4Event*);
        void add_step_energy(G4double);
    private:
        G4double event_erg;
        RunAction* ract;};
#endif
```

Listing A.12: EventAction.cc

```c++
#include "EventAction.hh"
EventAction::EventAction(RunAction* tmp)
    : G4UserEventAction() {ract = tmp;}
EventAction::~EventAction() {}
void EventAction::add_step_energy(G4double input) {event_erg += input;}
void EventAction::BeginOfEventAction(const G4Event* anEvent)
    { event_erg = 0.0;}
void EventAction::EndOfEventAction(const G4Event* anEvent){
    if (erg > 1.0e-20)
        ract -> add_event_energy(event_erg);}
```

pre- and post-step points. The steps with pre-step points inside the wax tank (the tally region) are selected, and the total deposited energy in these steps are accumulated to the event tally using the add_step_energy function defined in Listing A.12.

The Geant4 executable was compiled using the cmake utility. The calculated deposited energy in the paraffin tank is $0.938 \pm 1.20\%$, or between 0.927 to 0.949, MeV, which overlaps
Listing A.13: SteppingAction.hh

```cpp
#ifndef INCLUDE_STEPPINGACTION_HH_
#define INCLUDE_STEPPINGACTION_HH_
#include "EventAction.hh"
#include "G4UserSteppingAction.hh"
#include "G4Step.hh"
#include "G4StepPoint.hh"
#include "globals.hh"
class SteppingAction : public G4UserSteppingAction
{
public:
    SteppingAction(EventAction*);
    virtual ~SteppingAction();
    void UserSteppingAction(const G4Step*);
private:
    EventAction* eact;};
#endif
```

with the MCNP result of between 0.899 to 0.935 MeV.
#include "SteppingAction.hh"

SteppingAction::SteppingAction(EventAction* tmp)
: G4UserSteppingAction()
{ eact = tmp; }

SteppingAction::~SteppingAction() {}

void SteppingAction::UserSteppingAction(const G4Step* astep)
{
  // get step point
  G4StepPoint* pre_point = astep -> GetPreStepPoint();
  G4StepPoint* post_point = astep -> GetPostStepPoint();

  // get physical volume
  G4VPhysicalVolume* pre_pv = pre_point -> GetPhysicalVolume();
  G4VPhysicalVolume* post_pv = post_point -> GetPhysicalVolume();

  // get physical volume name
  G4String pre_name = "";
  G4String post_name = "";
  if (post_pv){
    pre_name = pre_pv -> GetName();
    post_name = post_pv -> GetName();
  }
  else
    return;

  // accumulate the deposited energy in the tank
  if (pre_name == "tank_pv"){
    G4double step_erg = astep -> GetTotalEnergyDeposit();
    if (step_erg > 1.0e-20)
      eact -> add_step_energy(step_erg);
  }
}
Appendix B

ElmerSolver Input

Shown below is a template ElmerSolver input written in a text sif file to calculate the electric field inside the MPFD gas volumes. Much of the contents are based on an official Garfield++ example [76]. While the inputs are self-explained, several notes are followed.

Check Keywords Warn

! mesh and output folder

Header

Mesh DB "." "FOLDER"

End

! Details of the calculation and output files.

Simulation

Coordinate System = Cartesian 3D
Simulation Type = Steady State
Steady State Max Iterations = 1
Output File = "FILE.result"
Post File = "FILE.ep"

End

! Define constants.

Constants
Permittivity Of Vacuum = 8.8542e-12

End

! Specify equation and material for gas.

Body 1
   Equation = 1
   Material = 1
End

! Define the ar gas

Material 1
   Relative Permittivity = 1.000516
End

! west wire

Boundary Condition 1
   Target Boundaries = 1
   Potential = 100
End

! east wire

Boundary Condition 2
   Target Boundaries = 2
   Potential = 0
End

! Details of the calculation procedure

Equation 1
   Active Solvers(1) = 1
   Calculate Electric Energy = True
End

Solver 1
   Equation = Stat Elec Solver
   Variable = Potential
Variable DOFs = 1
Procedure = "StatElecSolve" "StatElecSolver"
Calculate Electric Field = True
Calculate Electric Flux = False
Linear System Solver = Iterative
Linear System Iterative Method = BiCGStab
Linear System Max Iterations = 1000
Linear System Abort Not Converged = True
Linear System Convergence Tolerance = 1.0e-10
Linear System Preconditioning = ILU1
Steady State Convergence Tolerance = 5.0e-7
End

In the Header section, the folder with name FOLDER at current path that contains the ElmerGrid output files is specified. The ElmerSolver output result file is put into the same folder.

Body 1 is the physical gas volume defined in Gmsh. The governing equation 1 and material 1 (argon gas) are applied to this body. The governing equation and material are defined in the corresponding sections. The electrostatics solver for the governing equation is specified in the Solver section.

The applied voltages at the electrodes are specified in the boundary condition sections. The Target Boundaries keyword specifies the re-numbered physical surface identification number to which the boundary condition should apply. The Potential keyword specifies the applied voltage, i.e., 100-V voltage on anode and grounded cathode.
Appendix C

Electron Tracking in Parallel Plate

To examine the electron tracking simulation in Garfield++, a parallel-plate example was developed. A $2 \times 100 \times 100$ cm$^3$ box filled with argon gas at 1-atm pressure and 20 °C was modeled. A 100 V/cm constant electric field was applied in the gas volume along the positive $x$ direction. A 0.5 V/cm weighting electric field along the positive $x$ direction was set. Electrons were born at the center of the box. The Monte Carlo and the microscopic tracking algorithms were used to simulate the electron motion.

The electron trajectory and the induced current simulated by the Monte Carlo integration method are shown in Fig. C.1. The diffusion process was not considered. Under such conditions, the electron travels along the $x$ axis and traverses the 1-cm distance in approximately 4 $\mu$s. Thus, the electron drift velocity is about 0.25 cm/$\mu$s. It was reported that the mean drift speed for electrons in pure argon gas under an electric field $E$ and gas pressure $P$ can be approximated by [10]

$$v_e = \frac{3.64(E/P) + 114.6(E/P)^2}{1 + 12.7(E/P) + 304.33(E/P)^2} = 0.36 \text{ cm}/\mu\text{s} \quad (C.1)$$

for 100 V/s electric field and 1 atm (760 Torr) pressure. The difference may due to the facts that the mobility used in the Monte Carlo integration method was from a coarse electron transport table, and Eq. (C.1) is an approximation of the mean value. In the future work, the reason for this difference needs to be investigated.
To illustrate the effects of diffusion, the trajectories of five electrons and the induced current by tracking 50 electrons were simulated using the Monte Carlo integration and the microscopic tracking methods, and the results are shown in Fig. C.2. The results of these two methods are similar. The trajectories are much more random, and as a result, the induced current fluctuates.
Figure C.2: Trajectories of five electrons (a) and induced current of 50 electrons (b) simulated by the Monte Carlo integration method taking into consideration of the diffusion process. Using the microscopic tracking method, the trajectories of five electrons (c) and induced current by 50 electrons (d) are similar with the Monte Carlo integration results.