

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

**SIMULATION OF THE NEUTRON REFLECTION METHOD
USING GEANT4**



M.Sc. THESIS

Zehra GÜZEL

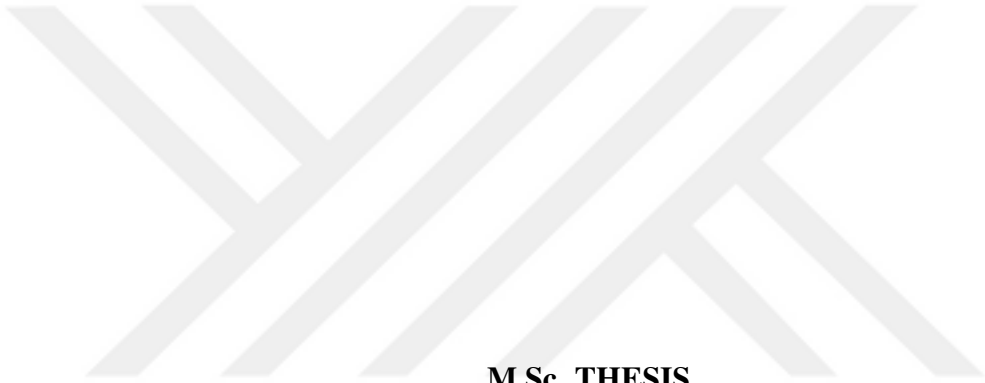
Nuclear Researches Division

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**Zehra GÜZEL
(302231009)**

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Thesis Advisor: Prof. Dr. İskender Atilla REYHANCAN

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

**GEANT4 KULLANARAK
NÖTRON YANSIMA YÖNTEMİNİN SİMÜLASYONU**

YÜKSEK LİSANS TEZİ

**Zehra GÜZEL
(302231009)**

**Nükleer Araştırmalar Anabilim Dalı
Radyasyon Bilim ve Teknoloji Programı**

Tez Danışmanı: Prof. Dr. İskender Atilla REYHANCAN

MART 2026

Zehra GÜZEL, a M.Sc. student of ITU Graduate School student ID 302231009 successfully defended the thesis entitled “SIMULATION OF THE NEUTRON REFLECTION METHOD USING GEANT4”, which she prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

Thesis Advisor : **Prof. Dr. İskender Atilla REYHANCAN**
Istanbul Technical University

Jury Members : **Prof. Dr. Cenap Şahabettin ÖZBEN**
Istanbul Technical University

Doç. Dr. Ayşe DURUSOY
Yıldız Technical University

.....

Date of Submission : **14 February 2026**

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To my family,



FOREWORD

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Zehra GÜZEL
(Physics Engineer)

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ABBREVIATIONS

BF₃	: Boron Trifluoride
BIC	: Binary Cascade model
Cd	: Cadmium
CDF	: Cumulative Distribution Function
CH₂	: Polyethylene
EBS	: Elastic Backscattering
EM	: Electromagnetic
G4	: Geant4 Class prefix
HP	: High Precision
MC	: Monte Carlo
NIST	: National Institute of Standards and Technology
OpenGL	: Open Graphics Library
Pu–Be	: Plutonium–Beryllium Neutron Source
QGSP	: Quark–Gluon String Precompound
QGSP_BIC	: Physics List Combining QGS with BIC
ROOT	: ROOT Data Analysis Framework



SYMBOLS

C	: Unit conversion constant (1 barn = 10^{-24})
d	: Sample thickness
E	: Neutron kinetic energy
$F(E_k)$	: Cumulative distribution function
I	: Thermal-neutron count rate with sample
I_0	: Thermal-neutron count rate without sample
m_n	: Neutron mass
m_p	: Proton mass
M	: Molecular mass
N	: Atomic number density (atoms·cm ⁻³)
N_A	: Avogadro's constant (mol ⁻¹)
n	: Total number of atoms in the sample
p_i	: Normalized sampling probability (spectrum bin i)
R	: Reflection ratio, $(I - I_0)/I_0$
s_{exp}	: Experimental uncertainty
s_{sim}	: Simulation uncertainty
s_i	: Combined uncertainty
$\sigma(E)$	: Microscopic cross section (barn)
σ_β	: Reflection cross section (barn)
$\Sigma(E)$	: Macroscopic cross section (cm ⁻¹)
λ	: Mean free path
χ^2	: Chi-square statistic
ν	: Degrees of freedom
δ_i	: Relative deviation
s_i	: Combined uncertainty
k	: Scaling factor
χ_v^2	: Reduced chi-square
Δ_i	: Point-wise difference
β	: Recoil Angle
θ	: Polar angle
ϕ	: Azimuthal angle
μ_N	: Nuclear magneton
MeV	: Megaelectron volt
eV	: Electron volt



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SIMULATION OF THE NEUTRON REFLECTION METHOD USING GEANT4

SUMMARY

Reactor physics, radiation shielding, non-destructive testing, and material characterization are just a few of the scientific and engineering disciplines that are supported by neutron interactions with matter. Because hydrogen has excellent neutron scattering and moderation capabilities, thermal neutrons are particularly effective in hydrogen-containing material. Because of this, thermal-neutron-based methods show a high degree of sensitivity to variables like the amount of moisture and the location of hydrogen in bulk materials.

The thermal-neutron reflection (albedo) approach is one useful method in this field. In the framework defined by Csikai and Buczkó, measurements are performed in a fixed source–moderator–detector arrangement. The detector response is compared in two cases: (1) without a sample and (2) with a sample placed near the detector. The reflection signal is expressed as the relative change in the thermal-neutron count rate and is commonly written as $R = (I - I_0)/I_0$, where I_0 is the reference count rate without the sample and I is the count rate with the sample [1]. From this response, the literature reports a reflection-related cross-section quantity (denoted here as σ_β). Csikai and Buczkó describe σ_β as a “semi-exact concept”: although it is given in cross-section units, it is not a purely microscopic material constant. Instead, it depends on the experimental setup, including the geometry, the moderation conditions, and how the detector response is defined. Therefore, a meaningful reproduction requires detailed modelling of both neutron transport and the measurement geometry.

This thesis reproduces the reference neutron-reflection setup [1] using the Geant4 Monte Carlo toolkit in a fully computational manner; no physical experiment is performed. Rebuilding the literature geometry in a contemporary transport code, comparing simulation results with published values for specific materials, and examining the sensitivity of low-energy neutron results to modeling decisions are the key objectives.

A fixed geometry model was constructed to represent the reference setup. The world volume was defined as vacuum. A polyethylene (CH₂) moderator was modelled with an internal cavity. A cadmium (Cd) shell was placed around the detector region. Because cadmium strongly absorbs thermal neutrons, this shell reduces unwanted direct thermal-neutron contribution and increases sensitivity to the intended reflection mechanism. The detector was represented by a simplified BF₃ sensitive volume. In relation to the moderator and detector, the sample was modeled as a disk-shaped target positioned at a fixed point. Only the sample material was altered during the simulation campaign, keeping the geometry constant so that variations in response could be ascribed to the material under the same measurement circumstances.

Primary neutrons were generated with a single-particle source producing neutron per event. To avoid directional bias, neutrons were emitted isotropically into 4π . The source was placed inside the moderator so that thermalization is driven by the geometry and the probability of direct streaming toward the detector is reduced. The initial neutron energy was sampled from an experimentally measured Pu–Be energy spectrum. The spectrum was discretized into energy nodes between 0 and 10.75 MeV, and the tabulated weights were normalized and used for random sampling. This approach aims to ensure that the implemented primary generator reproduces the intended input spectrum.

In this work, the detector response was defined without modelling electronics or pulse-height spectra. Instead, a simple and reproducible scoring definition directly linked to particle transport was used. Thermal-neutron counting was obtained with Geant4 command-based scoring using a scoring mesh defined independently of the mass geometry. A single-voxel mesh, “ThermalMesh,” was placed between the moderator and the sample. The scored quantity was the number of neutron track entries into this voxel. An energy filter selected thermal neutrons with kinetic energy up to 0.5 eV. For each material, two runs were performed: a “sample-out” run to obtain I_0 and a “sample-in” run to obtain I . The reflection signal was then computed and σ_β values were calculated using the same procedure for all materials.

Simulation outputs ($\sigma_{\beta,\text{sim}}$) were compared with published experimental values ($\sigma_{\beta,\text{exp}}$) for 43 materials. The dataset was grouped into three classes: elements ($n = 13$), inorganic compounds ($n = 14$), and organic compounds ($n = 16$). Agreement was evaluated using three complementary metrics: relative deviation, standardized residuals (z -scores) computed with the combined uncertainty, and a reduced chi-square statistic to summarize class-level consistency. This allowed differences to be assessed both at the material level (via $\Delta\%$ and z -scores) and at the class level (via χ^2).

The results show two clear patterns throughout the material groups. Only a small number of materials (large $|z|$) stand out in the simulation, which typically matches the experiment well for elements and inorganic compounds and follows an almost 1:1 trend. For organic compounds, the picture is different: the simulated values are lower than the experimental ones for almost all organics. However, while the simulations capture the general trend and ranking within the organic group, they remain at a lower scale. This is also reflected in the reduced chi-square values, which stay above 1 (especially for organics), meaning the raw simulation results do not fully agree with the experimental values within the combined uncertainties.

Overall, this study highlights that the extracted “reflection cross section” is an effective observable that depends on the setup. It is obtained from a scoring definition positioned between the moderator and the sample in Geant4. It depends on the moderated neutron spectrum, transport through surrounding volumes, multiple scattering inside the sample, and the probability that scattered neutrons enter the scoring region. Therefore, even small differences in spectrum/geometry weighting, finite-size effects, or sample-state assumptions can give noticeable residuals. Based on the results, it is recommended to (i) increase Monte Carlo statistics for the remaining outliers, (ii) test sensitivity to low-energy neutron physics of physics list options, (iii) re-check material definitions (composition, density, physical state), and (iv) verify stability against small changes in the scoring-mesh definition and key geometric parameters. These steps will improve the

consistency of the Geant4 model with experimental reflection observations by separating class-wide scale deviations from material-specific deviations.





GEANT4 KULLANARAK NÖTRON YANSIMA YÖNTEMİNİN SİMÜLASYONU

ÖZET

Nötronların madde ile etkileşimleri; nükleer reaktör fiziği, radyasyon zırhlama, tahribatsız muayene ve malzeme karakterizasyonu gibi birçok uygulamanın temelini oluşturur. Termal nötronlar, ortamla termal dengeye yaklaşmış ve oda sıcaklığında yaklaşık Maxwell dağılımı izleyen, karakteristik enerjisi $\approx 0.025\text{eV}$ mertebesindeki nötronlardır. Özellikle termal enerji bölgesindeki nötronlar, hidrojenin güçlü saçılma özellikleri ve yüksek moderasyon etkinliği nedeniyle hidrojen içeren ortamlara karşı belirgin duyarlılık gösterir. Bu durum, karmaşık malzemelerde nem miktarı veya hidrojen dağılımı gibi özelliklerin, termal-nötron alanındaki değişimler üzerinden dolaylı olarak izlenebilmesini mümkün kılar. Termal nötron yansıma (albedo) temelli yöntemler de bu yaklaşımın pratik örneklerinden biridir: sabit bir kaynak-moderator-dedektör geometrisi altında, termalleştirilen nötronların bir kısmını dedektör yönüne yansıtma eğilimi, ölçülebilir bir sayım artışına dönüşür.

Bu tez, literatürde tanımlanan Csikai-Buczkó nötron yansıma yöntemini Geant4 ortamında hesaplamalı olarak yeniden üretmeyi ve simülasyon ile yayınlanmış sonuçlar arasındaki uyumu nicel olarak değerlendirmeyi amaçlamaktadır. Yöntemde temel gözlenebilir büyüklük, örnek yokken ölçülen termal-nötron sayım hızı I_0 ile örnek varken ölçülen sayım hızı arasındaki farktan tanımlanan yansıma oranıdır: $R = \frac{I-I_0}{I_0}$. Bu yansıma oranından türetilen ve tez boyunca σ_β ile gösterilen yansıma kesiti, kullanılan moderasyon koşulları, ölçüm geometrisi ve dedektör yanıtının nasıl tanımlandığı gibi unsurlar tarafından belirlenen etkin bir parametredir. Dolayısıyla yöntemin güvenilir biçimde yeniden üretimi; yalnızca malzeme bileşiminin değil, aynı zamanda deneysel düzenin geometrik ayrıntılarının ve dedektör gözlenebilirliğinin açık şekilde modellenmesini gerektirir.

Tez kapsamında kurulan Geant4 modeli, ölçüm düzenini sabit tutacak şekilde yapılandırılmıştır. Bu çalışma, Monte Carlo parçacık taşınımına dayalı Geant4 kullanılarak gerçekleştirilmiştir. Geant4'te simülasyon; (i) deney düzeneğinin üç boyutlu geometrisinin ve malzemelerinin tanımlanması, (ii) birincil parçacık kaynağının ve enerji/açısal dağılımlarının örneklenmesi, (iii) seçilen fizik modelleri (physics list) ile etkileşimlerin adım adım taşınımının yapılması ve (iv) ilgi duyulan gözlenebilirlerin skorlama ile toplanması adımlarından oluşur. Dünya hacmi vakum olarak tanımlanmıştır. Moderatör, CH_2 malzemeden silindirik bir hacim olarak modellenmiştir; moderatör içinde deneysel düzende bulunan yerleşim boşluğunu temsil etmek üzere oyuk bölgesi boolean işlemlerle çıkarılmıştır. Dedektör bölgesi, oyuk içerisine yerleşecek biçimde tanımlanmış ve dedektörü çevreleyen kadmiyum (Cd) kılıf açık üst yüzeyli bir kılıf geometrisi olarak modellenmiştir. BF_3 dedektörün aktif bölgesi, duyarlı gaz hacmini temsil eden bir silindir olarak tanımlanmış; numune ise belirli yarıçap ve

kalınlığa sahip disk formunda tek tip bir hacim olarak kurulmuştur. Geometrik model ve örnek hacmi, literatürdeki düzeni takip edecek biçimde konumlandırılmıştır. Simülasyon boyunca geometri sabit tutulmuş; sistematik olarak yalnızca örnek malzemesi değiştirilmiştir. Böylece σ_β 'nin malzemeye bağlı davranışı, aynı ölçüm koşulları altında karşılaştırılabilir şekilde elde edilmiştir. Malzeme tanımları, mümkün olan durumlarda standart malzeme kütüphanesinden alınmış; kütüphanede doğrudan bulunmayan bileşikler ve karışımlar ise yoğunlukları belirtilerek kütle fraksiyonları üzerinden özel malzeme tanımları ile oluşturulmuştur. Bu sayede her numune için atomik sayı yoğunluğu ve makroskobik etkileşim davranışı, simülasyona tutarlı biçimde dâhil edilmiştir.

Birincil nötron üretimi, her olayda hızlı nötron üreten bir kaynak tanımıyla gerçekleştirilmiştir. Nötronlar 4π uzay açısına izotropik olarak yayımlanacak şekilde örneklenmiştir. Kaynak konumu moderatör bölgesi içinde seçilerek hem termalleşmenin etkin olması sağlanmış hem de dedektör yönüne doğrudan akı olasılığı azaltılmıştır. Başlangıç enerjileri ise deneysel olarak ölçülmüş bir Pu–Be nötron spektrumundan alınan ayrık enerji düğümlerinde örneklenmiştir. Spektrum, ağırlıkların olasılığa normalize edilmesi ve kümülatif dağılım fonksiyonunun oluşturulmasıyla, ters-dönüşüm örneklemesi üzerinden uygulanmıştır. Bu kaynak tanımı ile deneysel koşullara uyum amaçlanmıştır.

Dedektör yanıtı, elektronik/puls-yükseklik cevabı modellenmeden, Geant4'ün komut tabanlı skorlamasıyla tanımlanmıştır. Bu amaçla, kütle geometrisinden bağımsız olarak tanımlanan bir skorlama mesh'i kullanılmış ve moderatör ile örnek arasına tek voksel den oluşan bir “sanal dedektör” bölgesi yerleştirilmiştir. Gözlenebilir büyüklük olarak bu hacme giren nötron izlerinin sayısı (*track entry*) seçilmiştir; böylece sayım kavramı, belirli bir hacme giriş yapan parçacık sayısı üzerinden tekrarlanabilir bir şekilde tanımlanmıştır. Termal nötron seçimi için enerji filtrelemesi uygulanmış; $E_k \leq 0.5$ eV koşulunu sağlayan nötronlar sayım hesabına dahil edilmiştir. Her malzeme için iki ayrı koşu alınmış; örnek yok durumu I_0 , örnek var durumu I olacak şekilde yansıma oranı R hesaplanmış ve yansıma ile ilişkili kesit büyüklükleri (σ_β) tutarlı bir prosedürle elde edilmiştir.

Fizik tanımı, düşük enerjili nötron taşınımını güvenilir biçimde temsil etmek üzere modüler bir yaklaşımla kurulmuştur. Elastik saçılmada yüksek hassasiyetli (HP) düşük enerji nötron modelleri etkinleştirilmiş; hadronik inelastik süreçlerde geniş enerji aralığını kapsayan bir hadron modeli kullanılmıştır. İyon süreçleri, durdurma (stopping) mekanizmaları, foton–çekirdek etkileşimleri ve bozunma/radyoaktif bozunma süreçleri simülasyona dâhil edilmiştir. Çalışmanın odağı termal nötron davranışı olduğu için hesap yükünü kontrol etmek amacıyla elektromanyetik ikincil üretim belirli kesim (cut) ayarlarıyla baskılanmıştır. Buna karşın hadronik taşınımın ayrıntısı korunmuştur. Tüm malzemeler için aynı koşu ayarları ve aynı ölçüm tanımı kullanılarak, simülasyon sonuçlarının karşılaştırılabilirliği güvence altına alınmıştır.

Simülasyon çıktıları ($\sigma_{\beta, \text{sim}}$), literatürde yayımlanmış deneysel değerlerle ($\sigma_{\beta, \text{exp}}$) toplam 43 malzeme için karşılaştırılmıştır. Veri seti üç sınıfta ele alınmıştır: elementler ($n = 13$), inorganik bileşikler ($n = 14$) ve organik bileşikler ($n = 16$). Uyum değerlendirmesi üç tamamlayıcı metrikle yapıldı: yüzde hata ($\Delta\%$), standartlaştırılmış artık (z -skoru) ve indirgenmiş chi-kare (χ^2/N). Öncelikle her malzeme için deneysel

ve simülasyon belirsizliklerinin bağımsız olduğu varsayımıyla birleşik belirsizlik tanımlandı. Ardından malzeme bazında sapmanın büyüklüğü yüzde hata ile, bu sapmanın belirsizliklere göre anlamlılığı ise $z = (\sigma_{\beta, \text{sim}} - \sigma_{\beta, \text{exp}})/s$ ile değerlendirildi ve $|z| > 3$ koşulu birleşik belirsizlikle açıklanamayan uyumsuzluklar için eşik olarak kullanıldı. Son olarak sınıf düzeyindeki genel tutarlılığı özetlemek için her sınıf içinde $\chi^2 = \sum z^2$ toplanarak malzeme sayısına bölündü (χ^2/N). Böylece analiz, hem tek tek malzemelerdeki sapmaları ($\Delta\%$ ve z) hem de sınıf genelindeki uyumu (χ^2/N) aynı çerçevede ortaya koydu.

Sonuçlar, malzeme grupları arasında iki net örüntü olduğunu göstermektedir. Elementler ve inorganik bileşikler için simülasyon genellikle deneyle iyi uyuşmakta ve neredeyse 1:1 eğilimini izlemektedir; yalnızca birkaç malzeme (büyük $|z|$ değerleri) belirgin biçimde ayrılmaktadır. Organik bileşikler için ise tablo farklıdır: simüle edilen değerler, organiklerin neredeyse tamamında deneysel değerlerden daha düşüktür. Buna rağmen simülasyonlar organik grup içindeki genel eğilimi ve göreceli sıralamayı yakalamaktadır; asıl sorun doğru mutlak ölçeğin tutturulamamasıdır. Bu durum indirgenmiş chi-kare değerlerine de yansımaktadır: değerlerin 1'in üzerinde kalması (özellikle organikler için) hem simülasyon sonuçlarının birleşik belirsizlikler kapsamında deneysel değerlerle tam olarak uyuşmadığı anlamına gelir. Bu durum malzeme hatalarından ziyade sınıf düzeyinde bir ölçek kaymasına işaret etmektedir. Bu nedenle organikler için simülasyon kesitlerine tek bir ölçek faktörü uygulanmıştır: $\sigma_{\beta, s, i} = k \sigma_{\beta, \text{sim}, i}$. k değeri, birleşik belirsizlikleri dikkate alan ağırlıklı en küçük χ^2 yöntemiyle belirlenmiş ve ölçeklendirme sonrasında veriler 1:1 eğilimine önemli ölçüde yaklaşmıştır. Bu yaklaşım, organiklerdeki baskın ölçek farkını tek parametre ile düzeltirken, simülasyon belirsizlikleri de aynı çarpanla ölçeklenmiştir. Organik bileşiklerde yansıma kesiti, molekül başına hidrojen atom sayısı (n_H) ile güçlü pozitif korelasyon göstermiştir.

Genel olarak bu çalışma, elde edilen yansıma çapraz kesitinin düzeneğe bağlı etkin bir gözlenebilir olduğunu vurgulamaktadır. Bu büyüklük, Geant4'te moderatör ile numune arasına yerleştirilen bir skor tanımı (scoring mesh) üzerinden elde edilir. Moderasyonla oluşan nötron spektrumuna, çevre hacimler içinden taşınma, numune içindeki çoklu saçılmaya ve saçılan nötronların skor bölgesine girme olasılığına bağlıdır. Bu nedenle spektrum/geometri ağırlıklandırmasındaki küçük farklar, sonlu boyut etkileri veya numunenin fiziksel durumuna ilişkin varsayımlar bile belirgin sapmalar üretebilir. Ayrıca deneysel çalışmada numunelerin fiziksel durumu ve etkin yoğunluğu (toz/sıvı/katı, olası gözeneklilik) tam raporlanmadığından, simülasyondaki homojen kütle varsayımı bazı malzemelerde kalan uyumsuzluklara katkı yapabilir. Sonuçlara dayanarak şu öneriler sunulmaktadır: (i) kalan aykırı değerler için Monte Carlo istatistiğini artırmak, (ii) düşük enerjili nötron fiziği seçeneklerine duyarlılık testleri yapmak, (iii) malzeme tanımlarını (bileşim, yoğunluk, fiziksel durum) yeniden kontrol etmek ve (iv) skor mesh tanımındaki küçük değişimlere ve temel geometrik parametrelere (ör. organikler için numune yarıçapı) karşı sağlamlığı doğrulamak. Bu adımlar, sınıf düzeyindeki ölçek farkı ile malzeme bazlı sapmaları birbirinden ayırmayı sağlayarak, Geant4 modelinin deneysel yansıma gözlenebilirliği karşısındaki güvenilirliğini artıracaktır.



1. INTRODUCTION

Neutron interactions with matter play a central role in a wide range of scientific and engineering applications, including nuclear reactor physics, radiation shielding, non-destructive testing, and material characterization. In particular, thermal neutrons are highly sensitive to hydrogen-containing materials due to the strong scattering properties of hydrogen, making thermal-neutron-based techniques valuable for identifying moisture content and hydrogen distribution in complex samples. Among these techniques, neutron reflection methods provide an indirect but practical way to quantify how a material reflects moderated neutrons back toward a detector under a fixed source–moderator–detector geometry.

A classical approach to this problem was introduced by Csikai, who defined an effective quantity called the neutron reflection cross section (σ_β). This parameter aims to represent the ability of a material to “reflect” neutrons toward a detector, based on the difference between measured thermal neutron count rates obtained with and without a sample placed near the detector. Although σ_β is expressed in units of cross section, it is not a purely microscopic constant: it depends on the measurement configuration, the moderation conditions, and the detector response. For this reason, reproducing and interpreting reflection cross sections requires careful modelling of both neutron transport and experimental geometry.

Monte Carlo radiation transport codes provide an well-established framework for modelling neutron production, moderation, scattering, and detection under realistic conditions. In particular, Geant4 offers detailed physics models and evaluated nuclear data libraries that enable accurate treatment of low-energy neutron interactions, including thermal scattering interactions. Therefore, a Geant4-based reproduction of neutron reflection measurements can serve two purposes: (i) validating whether the method and reported results can be reproduced within a modern transport toolkit, and

(ii) providing insight into the sensitivity of σ_β to modelling choices such as physics lists, thermal scattering treatment, and geometric parameters.

This thesis presents a Geant4 simulation study that models the neutron reflection method described in the reference literature and compares the simulation-based results with reported reflection cross sections for selected materials. The study is designed as a computational reproduction and analysis; no physical experiment is performed within the scope of this thesis.

1.1 Purpose of Thesis

The primary purpose of this thesis is to reproduce the neutron reflection method reported in the literature using Geant4 and to evaluate the agreement between simulated and published reflection cross section values. To achieve this, a geometrical model representing the source–moderator–detector arrangement is constructed, and sample materials are introduced in accordance with the reference configuration. Thermal neutron detection is evaluated by a scoring methodology that mimics the detector response, and the reflection ratio is computed from simulated count rates with and without the sample.

The specific objectives of the thesis are:

- To implement a Geant4 model of the reference neutron reflection configuration, including the neutron source definition, moderation environment, sample placement, and detector representation.
- To compute the thermal-neutron count-rate change induced by different materials and to obtain the reflection ratio from simulation outputs.
- To derive simulation-based reflection cross sections and compare them with reported literature values for selected elemental and compound materials.
- To investigate the sensitivity of the results to modelling choices, including the selection of neutron high-precision (HP) physics models, thermal-scattering treatments, and geometric uncertainties.

Through addressing these objectives, the thesis aims to demonstrate how Monte Carlo modelling can support the interpretation of neutron reflection measurements and assess the reproducibility of reflection cross sections within a modern simulation framework.

1.2 Literature Review

Thermal neutron reflection (often described as neutron albedo or return probability) has been used for many years as a non-destructive way to characterize materials. It is especially useful for estimating hydrogen content, because hydrogen moderates neutrons and changes the thermal neutron field.

Early studies compared measurements with and without a reflecting sample. They often used activation foils to estimate how many thermal neutrons return, which created the basic idea of using reflection to distinguish materials.

In this approach, Csikai and Buczkó introduced the reflection cross section (σ_β). Instead of using only a large-scale albedo quantity, σ_β provides a microscopic, measurable parameter for thermal neutron reflection. For a fixed source–moderator–detector geometry, σ_β can be derived from the relative increase in detector count rate when a sample is present: $R = (I - I_0)/I_0$ and it can be related to the sample's areal density. However, σ_β is semi-empirical. It depends not only on the material, but also on the measurement setup (geometry). For dense materials and strong absorbers, σ_β can also saturate with thickness, meaning it stops increasing after a certain thickness.

A major experimental difficulty is flux depression inside the target, especially for materials with strong neutron absorbers. This can bias the σ_β value. To reduce this problem, Csikai and colleagues proposed using thin polyethylene (CH₂) foils as an internal flux monitor. They showed that the excess signal increases linearly with CH₂ thickness, and that the foil position inside the sample has only a small effect. They also reported that, under a fixed geometry, reflection cross sections are approximately additive for mixtures and compounds. This allows predictions based on composition. By defining an equivalent CH₂ thickness (using the CH₂ response as a reference), σ_β values can be calculated in a more consistent way across different samples in the same setup [2].

This reflection concept was later extended to include spectral information using fast-neutron elastic backscattering (EBS). Csikai and ElAgib showed that, for the broad Pu–Be spectrum, the measured backscattered spectrum can show energy-dependent features linked to elastic scattering from elements like C, N, and O. The total backscattered yield approaches saturation with increasing thickness, and hydrogen can reduce the effective volume being probed because it strongly moderates neutrons [3].

A related method (based on the same physics: moderation and thermal-flux changes) is activation-based hydrogen analysis in large samples. Dóczy et al. measured thermal-flux distributions in Cd-covered cylindrical samples using In and Dy activation foils. They defined an average flux and a relative excess flux parameter to quantify hydrogen effects. They reported strong correlations between the relative excess flux and total hydrogen content, and found that the average flux follows an exponential relationship on hydrogen concentration. Detector choice matters: in some ranges, Dy was more sensitive than In [4].

More recent studies have moved beyond laboratory tests toward applications such as industrial bulk analysis, soil moisture sensing, explosive/contraband detection, and screening where separating C/O/N/H is important. However, the reflection method is strongly affected by experimental conditions, including geometry, moderator thickness, neutron spectrum, and detector response. Therefore, σ_β values from experiments need careful validation and uncertainty analysis.

Because of this, Monte Carlo neutron-transport simulations have become very useful for reproducing reflection measurements, estimating uncertainties, and studying moderation and backscattering under controlled conditions. Among simulation tools, Geant4 is well suited for this because it includes detailed low-energy neutron physics using high-precision (HP) cross sections and thermal scattering models. This makes it possible to reproduce classical reflection experiments numerically and to separate the effects of geometry, material composition, and physics models, which is difficult to do experimentally.

In this thesis, the neutron reflection method in the Csikai framework is re-studied using Geant4. Simulated reflection ratios are used to calculate σ_β values for selected materials.

These results are then compared with literature data to check consistency and to study how sensitive σ_β is to key modelling choices.





2. THEORY

2.1 Introduction to Neutron Physics

Neutrons are electrically neutral hadrons. The neutron (n) has a rest energy of 939.566 MeV, charge 0, mass 1.0086649 u, spin 1/2, and a negative magnetic moment of about $-1.91 \mu_N$, where $\mu_N = \frac{e\hbar}{2m_p c}$ is the nuclear magneton and m_p is the proton mass. They do not interact with matter via Coulomb forces. They interact via the short range nuclear force or via magnetic interactions arising from their magnetic dipole moments. Neutrons generally exhibit large penetration depths in materials, and the probability of absorption is typically smaller than that of scattering. This makes scattering an important consideration in neutron measurements.

Neutron interaction probabilities depend strongly on neutron energy. The probability that a nuclear reaction occurs is expressed in terms of the concept of the cross section. The microscopic cross-section $\sigma(E)$ quantifies the probability of a particle interacting with a nucleus as it passes through a material. For example, the absorption cross-section expresses the probability of a neutron being absorbed within the material. Since this probability depends on the neutron energy, the cross-section is always considered as a function of E . The unit of microscopic cross section is barn. If there are N target nuclei per unit volume of the target material, the macroscopic cross section, $\Sigma(E)$ (unit: cm^{-1}), serves as an attenuation coefficient and is proportional to N (i.e., $\Sigma \propto N\sigma$). An important length scale is the mean free path, which is inversely proportional to the macroscopic cross section ($\lambda = 1/\Sigma$). It is the average distance a particle can travel before undergoing absorption or scattering.

Neutrons are mostly classified according to their kinetic energy. In fact, this classification was created to distinguish how neutrons interact with materials. A common distinction is thermal–epithermal–fast. Thermal neutrons are defined by a spectrum close to the Maxwell distribution at room temperature, with a peak around

0.025 eV. Epithermal neutrons are located above the thermal region, and Fast neutrons are typically evaluated in the 200 keV–10 MeV band. Above 10 MeV, they can be given as a separate class as high energy. Fast neutrons can be slowed down to slow and thermal neutrons with decelerating materials. The classification of neutrons according to their energy is as shown in Table 2.1.

Table 2.1: Classification according to neutron energy.

Classification	Energy Range
Cold neutrons	<0,003 eV
Thermal neutrons	0,003 eV- 0,4 eV
Epithermal neutrons	0,4 eV- 100 eV
Slow neutrons	100 eV - 200 keV
Fast neutrons	200 keV - 10 MeV
High energy neutrons	>10 MeV

2.1.1 Cross section

Neutron cross-sections are expressed in barns. One barn is equal to 10^{-24} cm^2 . One thousandth of a barn is called a millibarn and is denoted by mb. Elastic scattering is represented by the elastic scattering cross-section (σ_e), inelastic scattering by the inelastic scattering cross-section (σ_i), the (n, γ) reaction (radiative capture) by the capture cross-section (σ_γ), and fission by the fission cross-section (σ_f); and so on. As seen in equation (2.1), the sum of the cross-sections of all possible interactions is called the total interaction cross-section and is denoted by the symbol σ_t ;

$$\sigma_t = \sigma_e + \sigma_i + \sigma_\gamma + \sigma_f + \dots \quad (2.1)$$

The total cross-section measures the probability of any type of interaction occurring when neutrons strike a target. A neutron incident on a nucleus is either scattered or absorbed. The probabilities of scattering or absorption are given by the ratios of the corresponding scattering and absorption cross sections to the total cross section:

$$\sigma_t = \sigma_s + \sigma_a \quad (2.2)$$

In the definitions above, σ denotes the microscopic cross-section, i.e., the interaction probability per target nucleus, and it has units of area (barn). For a bulk material, interaction probabilities are more conveniently described by the macroscopic cross-section Σ (units: cm^{-1}), defined as $\Sigma(E) = N\sigma(E)$, where N is the atomic number density (cm^{-3}). Accordingly, the total macroscopic cross-section is $\Sigma_t = N\sigma_t$, and similarly $\Sigma_s = N\sigma_s$ and $\Sigma_a = N\sigma_a$. These quantities directly determine transport observables such as the mean free path, $\lambda = 1/\Sigma_t$, and attenuation in matter.

For bulk matter, it is convenient to use the macroscopic cross section $\Sigma_x(E)$ (cm^{-1}) defined as $\Sigma_x(E) = N\sigma_x(E)$, where N is the number density of target nuclei (cm^{-3}). For a compound, $\Sigma_x(E)$ is obtained by summing over all constituent species j as

$$\Sigma_x(E) = \sum_j \left(\frac{\rho N_A n_j}{M} \right) \sigma_{x,j}(E) \quad (2.3)$$

where ρ is the material density (g cm^{-3}), N_A is Avogadro's constant (mol^{-1}), n_j is number of atoms of element j in one molecule and M is the molecular mass.

Cross sections vary strongly with incident neutron energy and the target nuclide. Scattering cross sections are often approximately energy-independent (typically a few barns) over broad low-energy intervals, whereas absorption is larger for slow neutrons and may differ by several orders of magnitude across nuclides. Many absorption reactions follow an approximate $1/v$ trend in the thermal region ($\lesssim 1 \text{ eV}$). In the epithermal range, resonance peaks associated with compound-nucleus states are common, particularly for heavy nuclei. At higher energies, resonances increasingly overlap and the cross section becomes smoother on average, while channels such as inelastic scattering exhibit threshold behavior.

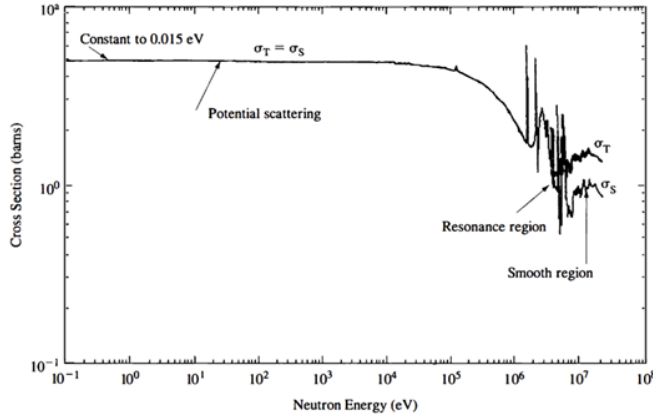


Figure 2.1: Elastic and total neutron cross sections of carbon versus neutron energy(eV; log scale).

Figure 2.1 shows the elastic and total neutron cross sections of carbon as a function of neutron energy. The plot highlights the potential-scattering plateau, the resonance region, and the high-energy smooth region [5].

2.1.2 Types of neutron interactions

A neutron with a given kinetic energy can, in many materials, penetrate more deeply than a charged particle of comparable energy (e.g., an α particle, electron/positron, or proton). This is primarily because neutrons are electrically neutral: they do not undergo continuous electromagnetic slowing via Coulomb interactions with atomic electrons, which dominate the stopping power of charged particles. Instead, neutrons lose energy through discrete nuclear interactions with target nuclei. [6] Depending on the interaction channel and neutron energy, a neutron may undergo scattering, transferring energy and momentum to the nucleus (with the nucleus recoiling), or it may be absorbed, leading to a nuclear transformation. Neutron–matter interactions are commonly grouped into scattering and absorption processes. Scattering comprises elastic scattering, in which the target nucleus remains in its ground state and the neutron’s energy reallocation is governed by two-body kinematics, and inelastic scattering, in which the nucleus is excited and subsequently de-excites, often by emitting one or more γ rays, while the outgoing neutron carries reduced kinetic energy. Absorption processes include radiative capture (n, γ), fission in fissile nuclides, charged-particle emission reactions (e.g., (n, p) , (n, α)), and multiple-neutron emission reactions (e.g., $(n, 2n)$, $(n, 3n)$)

when energetically allowed [5]. Figure 2.2 presents the classification of neutron–matter interactions into scattering and absorption processes.

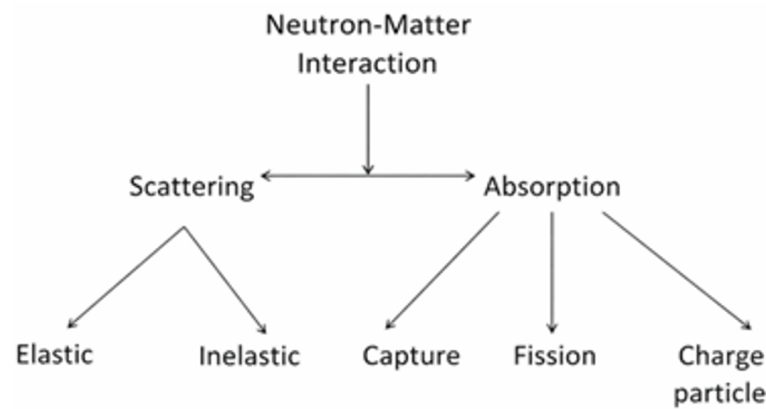


Figure 2.2: Neutron–matter interaction diagram.

Figure 2.3 shows the schematic representation of neutron–nucleus interactions: In elastic scattering, the neutron changes direction and exchanges energy and momentum with the nucleus, which recoils without excitation. In inelastic scattering, the neutron loses part of its energy during scattering, leaving the nucleus in an excited state that typically de-excites via gamma (γ) emission. In absorption (capture), the neutron is captured by the nucleus to form a compound nucleus, which may subsequently de-excite through γ emission or other radiation channels.

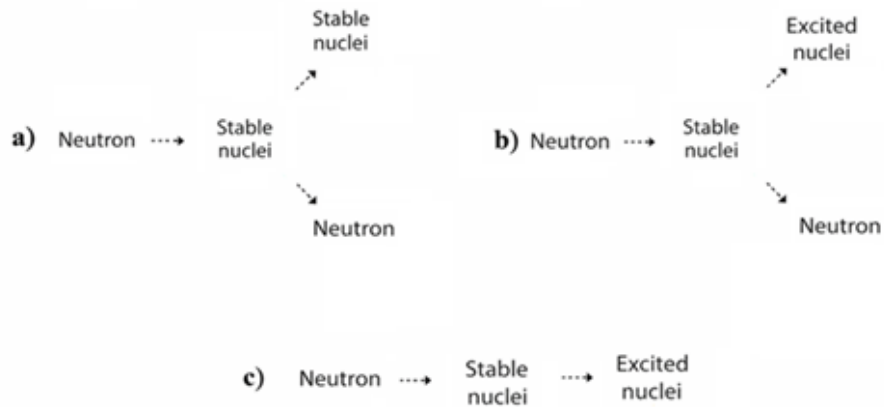


Figure 2.3: Schematic representation of neutron–nucleus interactions: (a) elastic scattering, (b) inelastic scattering, (c) absorption(capture).

2.1.2.1 Scattering

Elastic scattering (n, n) is a two-body interaction in which the incident neutron transfers part of its kinetic energy to a target nucleus while the nucleus remains in its ground state. With no internal excitation, the collision is purely elastic: momentum and energy are conserved, and the total kinetic energy remains constant in the non-relativistic regime relevant to neutron moderation. After the collision, the incident energy E_0 is redistributed between the scattered neutron (energy E') and the recoiling nucleus (recoil energy E_R), such that

$$E_0 = E' + E_R. \quad (2.4)$$

Elastic scattering therefore constitutes a main mechanism for slowing down (moderating) fast neutrons, particularly in low-mass-number media where large energy transfers per collision are possible. Geometrically, the incident neutron is scattered by an angle α relative to its original direction, while the target nucleus recoils at an angle β relative to the same reference axis. Let m_n be the neutron mass, M_t the target nucleus mass, and define the mass ratio $A = M_t/m_n$. The recoil energy (equivalently, the kinetic energy lost by the neutron in that collision) can be expressed in terms of the recoil angle β as,

$$E_R = E_0 \frac{4A}{(A+1)^2} \cos^2 \beta. \quad (2.5)$$

This relation shows that the energy transfer is maximal for a forward recoil ($\beta = 0^\circ$) and approaches zero as the recoil direction tends toward $\beta = 90^\circ$. The factor $\frac{4A}{(A+1)^2}$ also highlights why light nuclei are efficient moderators: for hydrogen ($A \approx 1$), the maximum transferable fraction approaches unity, whereas for heavy nuclei the maximum fraction is much smaller. Consequently, hydrogen-rich materials (e.g., light water and polymers such as paraffin or polyethylene) and other low- A moderators (e.g., graphite, heavy water) are widely used to reduce neutron energies from the fast to the thermal range [5].

Inelastic scattering ($n, n'\gamma$) is distinguished by excitation of the target nucleus. Linear momentum and total energy are conserved for the overall system; however, the kinetic energy of the outgoing particles is reduced because a portion of the incident kinetic energy is stored as nuclear excitation energy. The excited nucleus subsequently relaxes most commonly through the emission of one or more γ -rays while the scattered neutron exits with lower kinetic energy than the incident neutron. At higher incident energies, additional reaction channels (e.g., particle-emission reactions or fission, depending on the nuclide and reaction thresholds) may open. These processes are typically classified separately as non-elastic reactions rather than being treated as the standard ($n, n'\gamma$) inelastic-scattering channel [7].

2.1.2.2 Absorption

Since neutrons are uncharged, they are not repelled by a Coulomb barrier and can approach nuclei readily. In matter, slow neutrons undergo both scattering and absorption; elastic scattering is essential for slowing neutrons down, and as the neutron energy decreases the probability of absorption (often exhibiting $\sim 1/v$ behavior) generally increases, so neutrons in a finite medium will eventually be captured by nuclei. After absorption, a compound nucleus is formed with an excitation energy approximately equal to the neutron separation energy plus the incident neutron's kinetic energy (negligible for thermal neutrons). The compound nucleus typically de-excites by emitting prompt γ -ray cascades (radiative capture, (n, γ)), although for specific nuclides other absorption channels such as (n, p) or (n, α) can occur when energetically allowed [5]. These interaction mechanisms are schematically summarized in Figure 2.4, which illustrates the main reaction channels that may occur when an incident particle interacts with a target nucleus, including absorption, fission/spallation, radiative capture (γ emission), charged-particle production, and neutron production [8].

In charged-particle reactions, neutrons may also be removed via absorption reactions such as (n, p) and (n, α) , which can be exoergic or endoergic depending on the nuclide and Q -value. In neutron detectors, reactions like ${}^3\text{He}(n, p){}^3\text{H}$ and ${}^{10}\text{B}(n, \alpha){}^7\text{Li}$ are widely exploited because they produce energetic charged particles that ionize the detector gas (or the adjacent gas volume in converter-based designs), enabling pulse

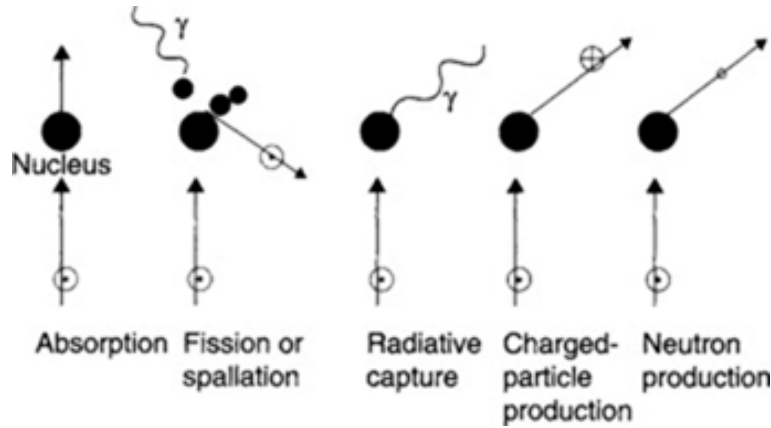


Figure 2.4: Schematic illustration of the main reaction channels.

formation and counting. The detectability of these channels is enhanced when the reaction products have sufficient range to deposit a measurable fraction of their energy in the sensitive volume.

Neutron-producing reactions of the type $(n, 2n)$ and $(n, 3n)$ require incident neutrons energetic enough to overcome the relevant neutron separation-energy constraints. Therefore, they are threshold reactions and are generally endoergic ($Q < 0$). The threshold energy depends on the target nuclide through separation energies and reaction kinematics. In practice, $(n, 2n)$ channels frequently open at energies on the order of several MeV (nuclide-dependent), whereas $(n, 3n)$ reactions typically require higher incident energies, often in the tens-of-MeV range, depending on the nucleus.

The neutron-induced fission occurs when an incident neutron is absorbed by a fissile or fissionable nucleus, forming an excited compound nucleus with mass number increased by one ($A \rightarrow A + 1$). The excitation energy of this compound system—approximately the neutron separation energy plus the incident neutron kinetic energy—may be sufficient to overcome the fission barrier, causing the nucleus to split into two fission fragments. This process is usually accompanied by the emission of prompt neutrons and prompt γ rays. The fragments are left highly excited and neutron-rich and subsequently de-excite through additional neutron/ γ emission (and later β decay). The outcome depends strongly on both the nuclide and the neutron energy. Fissile nuclides (e.g., ^{235}U , ^{239}Pu) can undergo fission with thermal neutrons, whereas many fissionable nuclides (e.g., ^{238}U) generally require fast neutrons above a threshold (of order MeV); consequently,

the fission probability can increase markedly with neutron energy for threshold-fission systems [5].

2.2 Neutron Sources

In the literature, neutron sources are generally classified according to how the neutron is produced: alpha-source systems operating via (α, n) reactions, spontaneously fissioning radionuclides, neutron-induced fission processes, photoneutron sources produced via (γ, n) reactions, sources based on charged particle accelerators, and fusion-based sources [9].

2.2.1 Alpha neutron sources

Alpha-particle excited neutron sources are among the most frequently used types of radioisotope-based neutron sources in the literature. In these sources, an α -emitting radioisotope is used together with a target, usually with a low atomic number (most commonly beryllium); neutron production occurs as a result of the interaction of the α particle with the target nucleus. An example of this is the reaction ${}^9\text{Be}(\alpha, n){}^{12}\text{C}$:



Since the energy released by the reaction is shared between the emitted neutron and the resulting ${}^{12}\text{C}$ nucleus, the neutrons produced do not have a single energy; instead, they exhibit a specific energy spectrum. The average energy of neutrons emitted from these sources is generally in the MeV range. Although various α -emitting radioisotopes can be used in practice, the choice of source depends on criteria such as half-life, radiation safety requirements, and the level of accompanying gamma emissions. Examples of commonly preferred α -emitters for this purpose include ${}^{241}\text{Am}$, ${}^{242}\text{Cm}$, ${}^{210}\text{Po}$, ${}^{239}\text{Pu}$, and ${}^{226}\text{Ra}$.

2.2.2 Spontaneous fission sources

Spontaneous fission is the unprompted (non-induced) breakup of a nucleus into two daughter nuclides (fission fragments), accompanied by the release of, on average, more

than one neutron. This process is characteristic of radionuclides with high mass numbers, typically $A \gtrsim 230$. Variations in the mass/scale distribution of fission fragments and the different number of neutrons released in each fission cause the energies of the produced neutrons to range approximately from 0 to 5.5 MeV [9].

2.2.3 Neutron-induced fission sources

Neutron-induced fission is the fundamental mechanism behind chain reactions in nuclear reactors and constitutes the primary source of high-flux neutron fields. Because multiple neutrons are produced in a single fission, the process can become a self-sustaining chain reaction. This is the basis for nuclear reactors being both a neutron and energy source. Since slow neutrons are required for efficient fission to occur at ^{235}U , moderators such as heavy water (D_2O) or graphite are used in reactors to slow down fast neutrons through elastic scattering.

2.2.4 Photoneutron (γ, n) sources

Photoneutrons are produced when sufficiently energetic photons induce (γ, n) reactions; the threshold depends on the neutron separation energy of the target nucleus. Beryllium is frequently used as a target because its photoneutron threshold is relatively low ($\approx 1.67 \text{ MeV}$), enabling radioisotope-based γ sources (e.g., Sb-Be) to generate neutrons [10].

2.2.5 Accelerator-based neutron sources

In accelerators, charged particles such as protons/electrons/deuterons are collided with a target; if the particles have sufficient energy, nuclear reactions occur with the target nuclei, and some can produce neutrons. In electron beams, bremsstrahlung photons are formed upon impact with the target; these photons interact with the nucleus (γ, n) and produce neutrons via the photoneutron mechanism. DeD/DeT (d, n) reactions in deuterons produce fast neutrons on the MeV scale (approximately 2.4 and 14.1 MeV) with high efficiency, even in small accelerators; at higher energies, very high-flux neutron fields can be obtained with spallation in heavy targets.

2.2.6 Nuclear fusion

Nuclear fusion occurs when nuclei combine at very high temperatures, transitioning into a plasma state and overcoming Coulomb repulsion; the energy released originates from mass defect/binding energy. The most important neutron-producing reactions are D–T and D–D fusions; the D–T reaction, in particular, releases 17.58 MeV of energy and produces fast neutrons of approximately 14.06 MeV. Therefore, controlled thermonuclear reactors are one of the main research areas for future energy production [5].

2.2.7 Pu–Be neutron source

In Pu–Be neutron sources, α -particles emitted by plutonium interact with ^9Be nuclei and generate fast neutrons via an (α, n) process. The reaction is typically expressed as



with a Q -value of about 5.7 MeV. The released energy, together with the incident α -particle energy, is shared between the outgoing neutron and the recoil nucleus, while additional energy may appear as γ -emission when ^{12}C is formed in excited states. The interaction is often described through the formation of an excited compound system (denoted $^{13}\text{C}^*$), which can decay through several competing channels, producing different combinations of ^{12}C final states and accompanying photons.

$$\alpha + ^9\text{Be} \rightarrow ^{13}\text{C}^* \rightarrow \begin{cases} n + ^{12}\text{C} + \gamma_1 & Q = 5.701 \text{ MeV} \\ n + ^{12}\text{C} + \gamma_1 & Q = 1.262 \text{ MeV}, h\nu_1 = 4.438 \text{ MeV} \\ n + ^{12}\text{C} + \gamma_1 + \gamma_2 & E_{\text{th}} = 2.821 \text{ MeV}, h\nu_2 = 3.216 \text{ MeV} \\ n + ^{12}\text{C} + \gamma_3 & E_{\text{th}} = 5.691 \text{ MeV}, h\nu_3 = 9.641 \text{ MeV} \end{cases} \quad (2.8)$$

This channel diversity, in the Equation 2.8, is the key reason why Pu–Be sources emit neutrons with a broadband energy distribution rather than a single discrete energy [6].

2.3 Neutron Detection Principles

Because neutrons are electrically neutral, they do not produce ionization in detector media through continuous Coulomb interactions in the same direct manner as charged particles. Neutron detection therefore relies predominantly on secondary charged particles and/or photons generated following a neutron interaction in either (i) a dedicated converter material or (ii) the detector medium itself. In practice, suitable reactions are selected to (a) provide an adequate interaction probability in the relevant energy range and (b) produce detectable secondaries with well-defined signatures. Commonly exploited channels include charged-particle-producing reactions such as (n, p) , (n, t) , and (n, α) ; fission reactions (n, f) in fissile converters; and capture reactions (n, γ) , which yield prompt γ -ray emission. From an instrumentation standpoint, neutron detection approaches are often grouped into [6] :

1. Prompt (real-time) methods, in which the neutron interaction generates an immediate electrical pulse (e.g., gas counters, scintillators, semiconductor devices with converters).
2. Delayed (activation-based) methods, in which neutrons are inferred from the decay radiation of activation products measured after irradiation (e.g., activation foils followed by γ -spectrometry).

2.3.1 Working principle of BF_3 proportional counter

BF_3 (boron trifluoride) detectors are gas-filled proportional counters, usually built as cylindrical metal tubes with a central anode wire. The fill gas has two roles: it collects ionization charge and it converts neutrons through boron, mainly the ^{10}B isotope, via the thermal-neutron reaction:



For thermal neutrons, this reaction has two main branches. In the dominant branch, ^7Li is produced in an excited state and then emits a 0.478 MeV γ ray:

$$^{10}\text{B} + n \rightarrow ^7\text{Li}^* + \alpha \quad (2.10)$$

$$^7\text{Li}^* \rightarrow ^7\text{Li} + \gamma(0.478\text{MeV}) \quad (2.11)$$

A smaller fraction goes directly to the ground state without γ emission. For thermal neutrons, typical branching fractions are about 94% (γ -emitting) and 6% (no γ).

After capture, the α particle and the ^7Li recoil are emitted roughly in opposite directions (the incident thermal-neutron momentum is usually negligible). As these charged particles move through the BF_3 gas, they lose energy mainly by ionization and create electron-ion pairs. The electric field drives the electrons toward the anode wire. Near the anode, the field is strong and causes gas multiplication. This produces an output pulse. In proportional operation, the pulse height is roughly proportional to the energy deposited in the gas.

Therefore, the pulse-height spectrum depends on both reaction kinematics and detector geometry. In practice, it is strongly affected by the wall effect. If the range of a reaction product is comparable to the tube dimensions, the particle may hit the wall before stopping in the gas. Then part of its energy is deposited in the wall instead of the gas. This reduces the measured pulse height and creates a continuum toward lower pulse amplitudes [6].

2.4 Bulk Analysis and Neutron Reflection Method

Bulk analysis refers to measurement methods that probe a representative volume of a sample (not only the surface) and infer an average material property or composition from the detected signal. In neutron-based bulk analysis, hydrogen is especially important because it strongly affects neutron moderation and, as a result, changes the neutron field in a measurable way [11,12].

In this thesis, the thermal neutron reflection (albedo) method is treated as a neutron-based bulk analysis technique. The basic idea is that neutrons thermalized in a moderator enter the sample, undergo scattering, and a fraction of them return toward

the detector region. Therefore, adding a reflecting sample increases the measured count rate compared with the “no-sample” condition.

A key aspect of the approach by Csikai et al.(1999) is to describe thermal neutron reflection not only with a macroscopic “albedo” concept, but also with a microscopic parameter, commonly called the reflection cross section (denoted here by σ_β) [1]. Importantly, σ_β is not a universal material constant: it depends on the sample composition and also on the measurement geometry. However, when the source–moderator–sample–detector configuration is kept fixed, σ_β provides a consistent basis for comparing the thermal reflection behavior of different materials. The experimental reflection signal is expressed as the relative change in the detector response:

$$R = \frac{I - I_0}{I_0} \quad (2.12)$$

where I is the measured count rate with the sample present and I_0 is the count rate in the reference configuration without the sample. In the Csikai formulation, the relative reflection signal is related to σ_β through the sample’s atom density and dimensions:

$$R = CNd\sigma_\beta = C \frac{n\sigma_\beta}{S}. \quad (2.13)$$

In this expression, n denotes the total number of atoms in the sample, N is the atomic number density (atoms/cm³), S is the illuminated sample surface area (cm²), and d is the sample thickness (cm). The factor C is a unit conversion constant—commonly taken as $C = 10^{-24}$ so that σ_β is obtained in barns. Solving for σ_β gives:

$$\sigma_\beta = \frac{RS}{Cn} \quad (2.14)$$

This provides a direct pathway from measured count rates (I, I_0) to a single parameter (σ_β) that characterizes thermal neutron reflection under the chosen experimental geometry. For compounds, a molar form of the reflection cross section can be introduced by assuming that the molecular response can be approximated as the sum of contributions from the constituent atoms:

$$\sigma_{\beta,\text{mol}} = \sum_i n_i \sigma_{\beta i} \quad (2.15)$$

where n_i is the number of atoms of type i in the molecule. The validity of this additivity approximation is typically discussed together with thickness effects; for many practical sample types, the atomic reflection response is reported to remain approximately constant up to about the centimeter scale, whereas deviations may occur for certain metals and for strongly absorbing materials [1,4].

Therefore, this thesis uses the reflection method because, with a fixed geometry, it provides a measurable σ_{β} that can be compared. Its limitations are discussed in the uncertainty analysis and discussion sections.

2.5 Monte Carlo Methods and GEANT4

Monte Carlo (MC) methods are a class of computational techniques that estimate physical quantities by repeated random sampling of probabilistic models [13]. In radiation and particle-transport problems, the principle physics can be expressed in terms of interaction probabilities (e.g., cross sections, angular distributions, and energy-loss laws), and MC simulation proceeds by generating many independent particle histories whose interactions are sampled from these distributions. Ensemble averages of the simulated histories yield estimators for observables including particle fluence, energy deposition, or detector response, while the statistical uncertainty of such estimators typically decreases with the number of (uncorrelated) simulated histories, scaling approximately as $1/\sqrt{N}$ [14].

In practical transport simulations, an MC code tracks particles through a specified geometry and material composition by sampling the distance to the next interaction (or boundary) and selecting the reaction channel when an interaction occurs; secondary particles are then generated and tracked when reactions produce them. This event-by-event approach is especially valuable when the problem includes complex three-dimensional geometries, mixed materials, and coupled physics (electromagnetic and hadronic interactions, decay chains, and secondary production), where deterministic methods may become difficult to apply without strong approximations [13].

Geant4 is a widely used, object-oriented Monte Carlo toolkit designed for simulating the passage of particles through matter. It provides a comprehensive software framework for defining detector geometry and materials, generating primary particles, tracking particles through fields and volumes, and modeling a broad range of physics processes (electromagnetic, hadronic, and optical, among others) over a wide energy domain. The toolkit is structured so that users build an application by selecting or composing appropriate physics models (often through predefined physics lists), implementing sensitive detectors and scoring, and customizing simulation control via user actions (e.g., run/event/step-level hooks). This modular design supports transparent configuration, reproducibility, and extensibility for research applications spanning high-energy physics, medical physics, space-radiation studies, and radiation protection [15].

Geant 4's software structure is summarized by the top-level category diagram (see Figure 2.5). The diagram mainly shows how the main Geant4 modules depend on each other, and it is designed to avoid circular dependencies. In the Figure 2.5, an open circle on a connecting line indicates a uses relationship: the category at the circle end uses the adjacent category. At the base level, Geant4 provides common services through modules such as global, materials, particles, geometry (including navigation), and intercoms. Particle transport is then organized around track, processes, and tracking. The track category defines tracks and steps, processes implement the physics interactions (including transportation through the geometry), and tracking manages how these processes act on a track during its evolution. At a higher level, the event category manages events in terms of their tracks, and the run category manages collections of events that share the same beam and detector setup; readout supports handling of pile-up. Finally, visualization, persistency, and interfaces provide ways to connect Geant4 outputs to external tools for graphics and data storage [15].

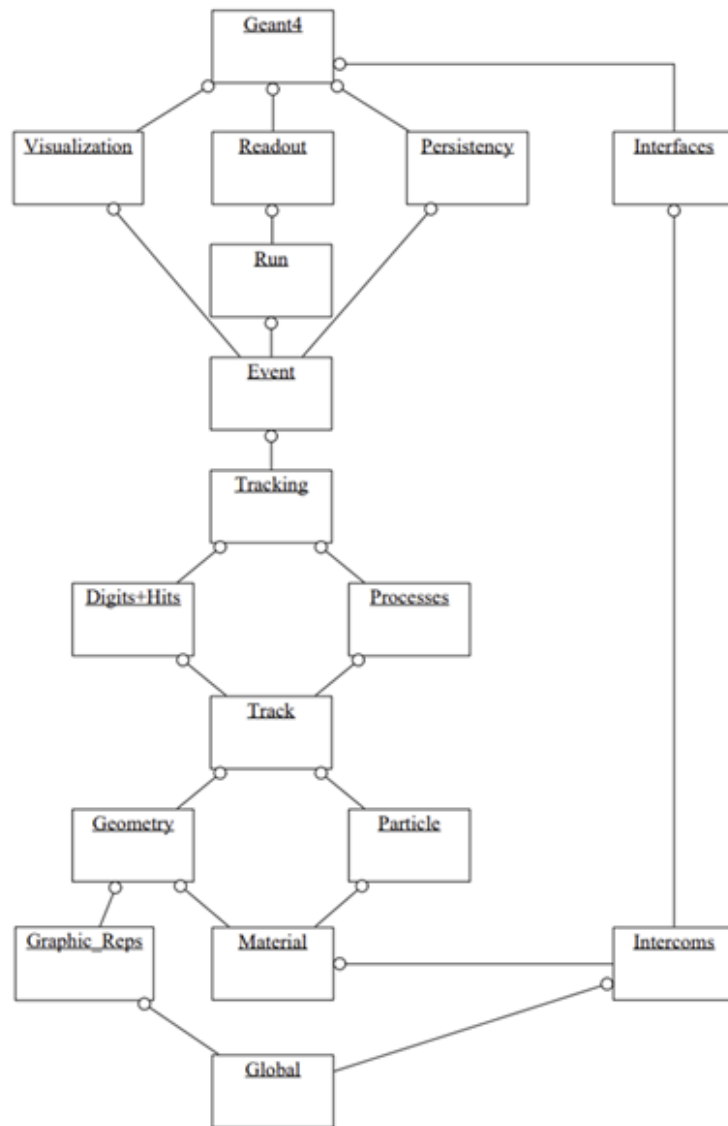


Figure 2.5: Top-level category diagram of Geant4 illustrating the main functional modules and their dependencies.

In the present study, the measurement setup was implemented by defining the full 3D geometry and material composition within the detector construction stage, configuring the primary particle source, and selecting an appropriate physics configuration for neutron transport. The quantities of interest (e.g., thermal-neutron counts/fluence in a specified region) were obtained via scoring, providing a virtual measurement definition that is decoupled from detector electronics while remaining fully consistent with the event–track transport kernel.



3. GEANT4 SIMULATION MODEL

In this section, the thermal neutron reflection (albedo) measurement geometry defined by Csikai and Buczkó is modelled within the Geant4 framework, and the measurement principle of the method is numerically reproduced. In the approach proposed by Csikai and Buczkó, the concept of the reflection cross section (σ_β) is sensitive not only to the composition of the sample, but also to the source–moderator–detector–sample arrangement and the resulting thermal neutron field generated by this configuration [1]. Therefore, throughout the simulation campaign, the measurement geometry was kept fixed, while only the sample type was varied systematically. The model includes (i) geometry, (ii) material definitions, (iii) source and spectrum, (iv) scoring, and (v) physics/run settings. In the following subsections, we describe how each component is implemented in the Geant4 model and detail how the ratio $R = \frac{I-I_0}{I_0}$ and the corresponding σ_β outcome is obtained from the count-rate observables (without sample) and I (with sample). Figure 3.1 presents a visualization of the simulated geometry as rendered using the Geant4 OpenGL interface. Wireframe outlines indicate volume boundaries, while axis markers and scale bars (30 cm) define the global coordinate system.

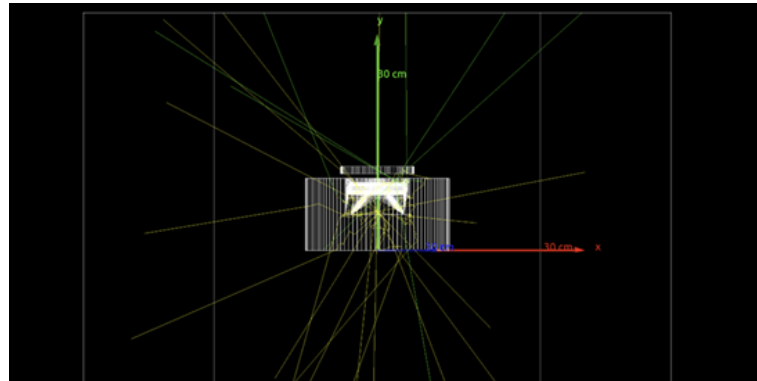


Figure 3.1: Visualization of the simulation geometry.

3.1 Geometric Model

In Geant4, accurate definition of the detector geometry is one of the key steps determining the physical realism of a simulation. In this study, the experimental setup was modelled in accordance with the measurement geometry proposed by Csikai et al., reproducing the source–moderator–detector–sample configuration used in the laboratory. All geometric components and their placements were implemented within a user-developed Detector Construction class. The geometry construction followed Geant4’s three-level approach: each component was first defined as a solid geometry (`G4VSolid`) specifying its shape and dimensions, then converted into a logical volume (`G4LogicalVolume`) where material and volume properties were assigned, and finally positioned within the world volume using physical volumes (`G4VPhysicalVolume`; e.g., `G4PVPlacement`) carrying the appropriate position and rotation information.

To model structural details such as cavities and coatings present in the Csikai measurement assembly, Boolean operations were employed [1]. In particular, `G4SubtractionSolid` was used to create cut-outs and void regions, while `G4UnionSolid` was applied where the combination of multiple shapes was required. The orientations of individual components consistent with the experimental geometry were defined using `G4RotationMatrix`. The world volume was defined as a cubic box filled with vacuum (“Galactic”), with half-length $fWorldSize=33$ cm. Detector Construction class implemented for the purposes of this thesis is presented in Appendix C.

The moderator and cavity were modelled as a polyethylene (CH_2) cylinder (`G4Tubs`) with radius $R = 10$ cm and half-length $L/2 = 5$ cm, placed at $(0, 5.0\text{ cm}, 0)$. The cylinder was rotated by 90° about the global X axis such that its symmetry axis aligns with the global Y direction. A rectangular cavity was carved out using a subtraction solid to reproduce the experimental insertion region. The cavity half-dimensions were set to $X = 4.2\text{ cm}$, $Y = 1.35\text{ cm}$, and $Z = 2.5\text{ cm}$ and shifted along the moderator axis by $+2.5\text{ cm}$ so that the cavity opens from the top face of the moderator, enabling the

placement of the cadmium shell and the detector. The moderator is a defined block volume of CH_2 material used to slow down fast neutrons into the thermal energy region. In Figure 3.2, the moderator volume is shown in blue region.

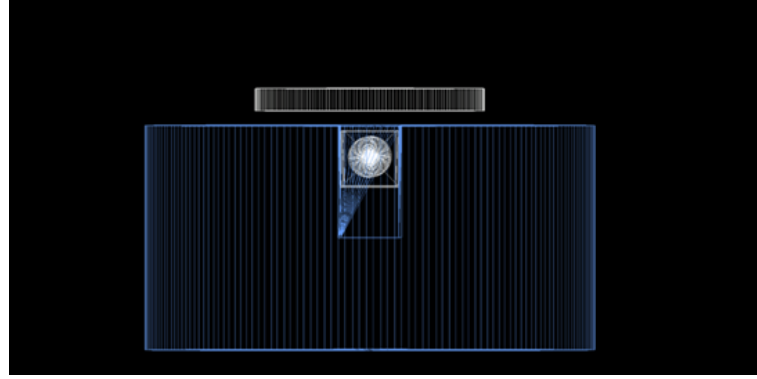


Figure 3.2: OpenGL view of the source–moderator–detector setup in Geant4. The blue region denotes the CH_2 moderator volume.

A cadmium open-top box was implemented as a hollow rectangular shell (G4Box–subtraction) with wall thickness $t = 0.5$ mm. The outer half-dimensions were $X = 4.1$ cm, $Y = 1.25$ cm, and $Z = 1.25$ cm. The inner void was shifted by $+t$ along the local Z direction to keep the top face open while leaving a bottom base. As shown in Figure 3.3, the shell was placed at $(0, 8.5 \text{ cm}, 0)$ with the same 90° rotation about X as the moderator, ensuring consistent alignment with the cavity. Because cadmium strongly absorbs thermal neutrons, it effectively determines the energy range over which the measurement is sensitive. Placing Cd around the detector reduces the direct impact of thermal neutrons generated in the moderator on the detector; this helps to make the measurement more sensitive to the targeted mechanism [16].

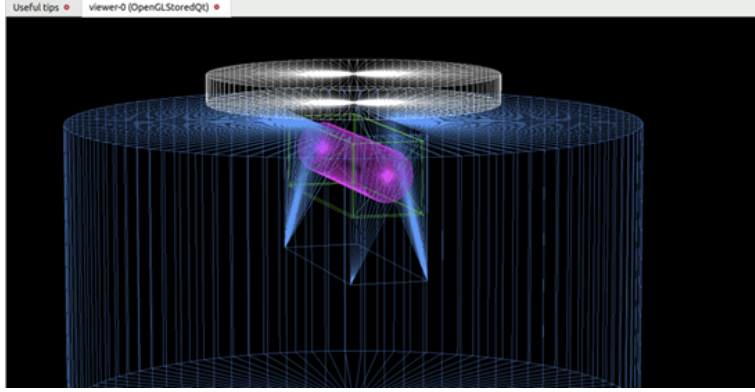


Figure 3.3: OpenGL view of the source–moderator–detector setup in Geant4. The green box denotes the cadmium (Cd) shell surrounding the detector.

The BF_3 detector model was represented by a cylindrical gas volume (`G4Tubs`) filled with enriched BF_3 gas. The active volume radius was set to $R = 0.9\text{ cm}$ and the half-length to $L/2 = 4.0\text{ cm}$ (corresponding to an 80 mm active length). The detector was rotated by 90° about the global Y axis to align the tube axis with the global X direction, and it was positioned at $(0, 8.6\text{ cm}, 0)$ so that it sits inside the cadmium shell within the moderator cavity (see Figure 3.4).

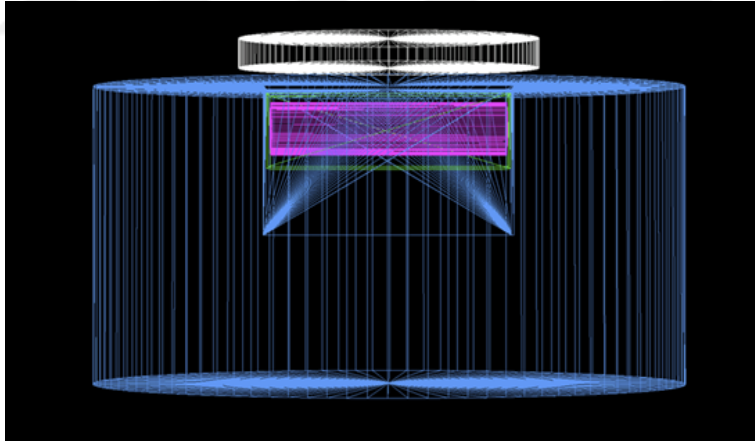


Figure 3.4: Geant4 OpenGL view of the detector volume modeled as an 8 cm pink cylinder.

The sample geometry was modelled as a cylindrical disk with radius $R = 5.1\text{ cm}$ and half-thickness $d/2 = 0.5\text{ cm}$ (1 cm total thickness in the baseline geometry), placed at $(0, 11.15\text{ cm}, 0)$ and rotated by 90° about the global X axis. The white cylinder in the Figure 3.4 represents the sample volume located above the moderator.

Neutrons were generated from a point source positioned at (0, 5.4 cm, 0), i.e., within the moderator region. Placing the source outside the cadmium-lined box also avoids direct streaming into the detector region and helps ensure that the measured response is dominated by moderated and reflected neutrons. The energy sampling procedure and the adopted neutron energy distribution are described in Section 3.3.

3.2 Material Definitions

All materials used in the simulation were defined within Geant4 using the standard Geant4 material classes. The material set was established in the `DetectorConstruction` class by combining (i) reference materials obtained via `G4NistManager` and (ii) custom-defined materials created from elements and isotopes when a specific composition was required. Material densities were assigned according to literature values or standard reference definitions, depending on the material type and availability.

3.2.1 Standard materials (NIST database)

Whenever possible, elemental and compound materials were retrieved using `G4NistManager::FindOrBuildMaterial()`. This ensured consistent baseline properties for commonly used materials in the geometry (e.g., structural metals and standard compounds) and minimized ambiguity in material specification.

3.2.2 Custom compounds and mixtures

For materials not directly available as predefined entries, custom materials were constructed using `G4Material` by specifying the density and adding constituents using either:

- Stoichiometric definitions (fixed atom ratios) for well-defined compounds (e.g., CH_2 , BF_3), or
- Mass-fraction definitions for mixtures specified in weight percent.

This approach preserves the intended composition while providing the macroscopic material properties required by particle transport and interaction processes. A complete list of defined materials and input densities is provided in Appendix A.

3.3 Source Definitions and Energy Spectrum

A mono-particle primary generator was implemented using the `G4ParticleGun` in Geant4. Each event generates a single neutron primary. The neutron source was modelled as a point emitter located at $(x, y, z) = (0, 5.4 \text{ cm}, 0)$, i.e., within the moderator region in the fixed Csikai–Buczkó measurement geometry [1].

Neutrons were emitted isotropically into 4π . The direction unit vector was sampled from a uniform distribution in solid angle by drawing $\cos \theta \sim U(-1, 1)$ and $\phi \sim U(0, 2\pi)$, and constructing $\vec{u} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. This choice ensures an unbiased, geometry-driven establishment of the thermal neutron field in the geometry configuration.

The initial neutron energy was sampled from a tabulated Pu–Be spectrum discretized into energy nodes between 0 and 10.75 MeV. Let E_i denote the energy nodes and w_i the corresponding (unnormalized) spectral weights. The weights were normalized to probabilities

$$p_i = \frac{w_i}{\sum_j w_j}, \quad \sum_i p_i = 1 \quad (3.1)$$

and the cumulative distribution function (CDF) was constructed as

$$F(E_k) = \sum_{i \leq k} p_i \quad (3.2)$$

For each primary, a uniform random number $r \sim U[0, 1)$ was generated and the sampled energy was obtained by inverse-transform sampling: the first energy node E_k satisfying $F(E_k) \geq r$ was selected. In the present implementation, energies are sampled discretely at the predefined nodes (i.e., without interpolation between adjacent points), reproducing the adopted tabulated spectrum as encoded in the Primary Generator class. The full table of Pu–Be energy nodes and normalized weights is provided in Appendix B.1, while the

implementation of the `PrimaryGeneratorAction` class is given in Appendix D. Figure 3.5 presents the experimentally measured Pu–Be neutron energy spectrum used as the input distribution to sample primary neutron energies in the Geant4 simulations. The primary neutron energies were sampled from this experimentally measured Pu–Be spectrum [17]. Figure 3.6 shows the corresponding neutron energy spectrum at particle generation, confirming that the implemented sampling reproduces the intended input shape.

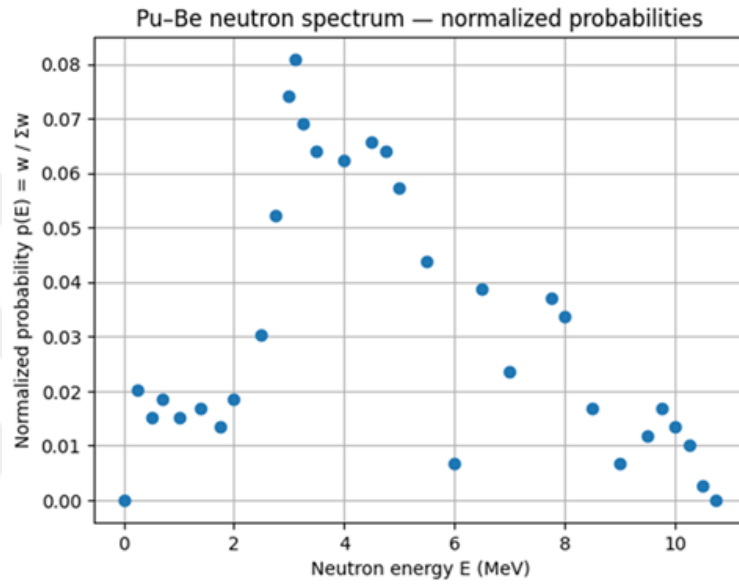


Figure 3.5: Normalized experimental Pu–Be neutron energy spectrum.

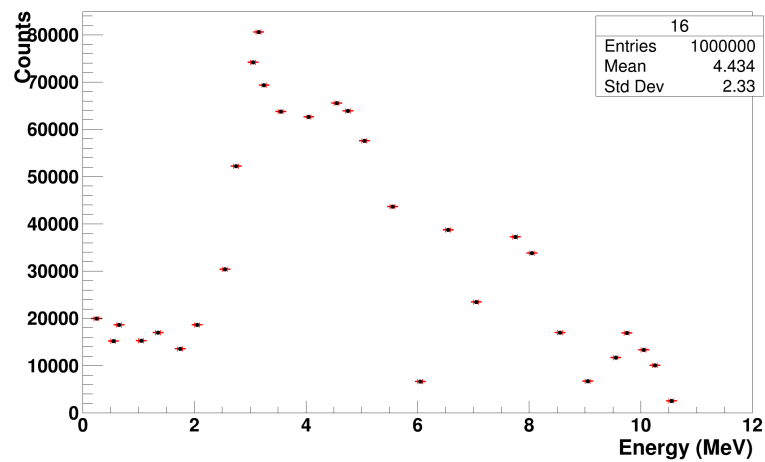


Figure 3.6: Primary neutron energy spectrum at particle creation obtained in Geant4 ROOT analysis when the predefined Pu–Be source spectrum is used in the particle generator.

3.4 Scoring Methodology

Thermal-neutron counting in the detector region was obtained using Geant4's command-based scoring with a scoring mesh. In command-based scoring, Geant4 assigns a `G4MultiFunctionalDetector` to a scoring volume that can be either (i) a logical volume in the tracking (mass) geometry or (ii) a volume created in a dedicated parallel world (e.g., a scoring mesh or probe). During tracking, primitive scorers attached to this scoring volume accumulate run-level scores, which are automatically merged across worker threads at the end of the run [18].

A scoring mesh can be defined with box or cylinder geometry, where mesh dimensions are specified as half widths (consistent with `G4Box/G4Tubs`). The mesh can be translated/rotated and subdivided into bins, and it is defined independently of the mass geometry. Here, a single-voxel `ThermalMesh` was used (`nBin 1 1 1`). With `boxSize (5.2, 0.2, 5.2)` cm given as half widths, the physical mesh size is $10.4 \times 0.4 \times 10.4$ cm, and it was placed at `translate/xyz 0 10.63 0` cm in the detector region between the source line and the sample position.

The primitive scorer `volumeFlux` was used because it scores the number of tracks getting into the volume, which directly matches the intended “counts” through the virtual detector region. Thermal neutrons were selected using a `particleWithKineticEnergy` filter, accepting only neutrons with kinetic energy in $0\text{--}5 \times 10^{-7}$ MeV (i.e., 0–0.5 eV). In command-based scoring, the `/score/filter` command applies to the immediately preceding scorer; therefore, the energy filter was attached to the `volumeFlux` scorer (`Npass`). Two separate runs were performed for the sample-out and sample-in configurations. An example of the scoring macro used in this study is provided in Appendix E. The resulting scores were used to compute the relative change $R = (I - I_0)/I_0$ and to derive reflection-related quantities from the difference between the two condition. Figure 3.7 illustrates the placement of the scoring mesh relative to the simulation geometry.

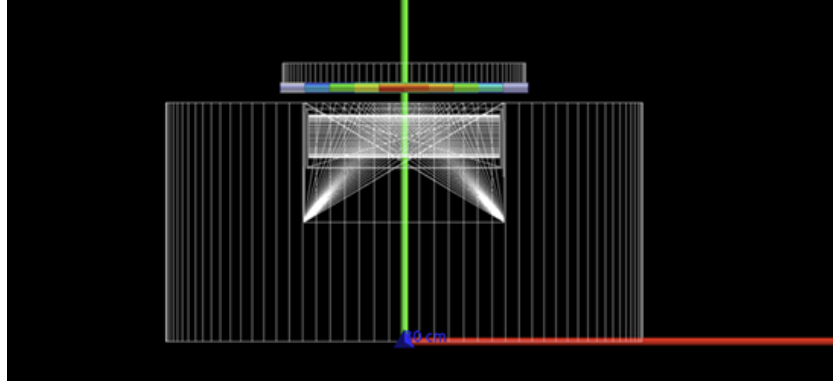


Figure 3.7: ThermalMesh scoring mesh (single voxel) positioned between moderator and sample.

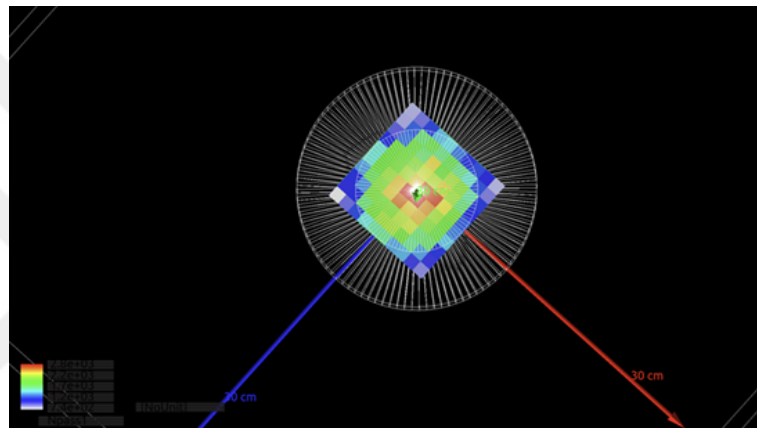


Figure 3.8: Visualization of scoring mesh heat map

Figure 3.8 shows the scoring mesh heat map of neutron volume flux obtained from the Geant4 simulation, where warmer colors indicate higher flux values and cooler colors represent lower flux regions.

3.5 Physics List Selection

The physics list used in this study was defined using a modular approach, combining models that describe both low-energy neutron behavior and general particle–matter interactions within a single configuration. The following physics components were activated:

- **Hadronic elastic scattering (HP approach):** To model low-energy neutron elastic scattering with improved fidelity, a High Precision (HP) elastic module

was employed. This choice is intended to increase the material-dependent accuracy of neutron transport, particularly in the thermal/epithermal energy range.

- **Hadronic inelastic processes (QGSP_BIC):** Hadron inelastic interactions were handled using the QGSP_BIC hadronic model, which provides a widely used framework covering hadron–matter reactions over a broad energy interval.
- **Ion processes:** Dedicated modules for ion elastic and ion inelastic interactions (including a cross-section–driven ion model) were included to represent the transport of heavy charged particles in a consistent manner.
- **Stopping physics:** Stopping processes were enabled to account for absorption and related mechanisms affecting low-energy charged particles.
- **Photon–nucleus interactions:** Gamma-nuclear processes were activated to represent photon-induced nuclear reactions, including secondary production where applicable.
- **Electromagnetic processes:** A study-specific electromagnetic physics module was assigned so that EM interactions are treated within the selected modeling framework.
- **Decay processes:** Standard particle decay and radioactive decay were enabled together to ensure consistent handling of unstable species.

Production cuts were adjusted in accordance with the primary simulation objective. In the current configuration, the cut value for protons was set to 0 mm to preserve hadronic tracking detail, whereas the cuts for e^- , e^+ , and γ were set to a very large value (10 km) to strongly suppress electromagnetic secondary production. This setting is treated as a computational optimization when the main focus is on particle transport (e.g., neutron behavior) rather than detailed electromagnetic cascade development [19].

3.6 Methodology

3.6.1 Data sources and reported quantities

The experimentally reported reflection cross sections $\sigma_{\beta_{\text{exp}}}$ and their uncertainties ($\pm s_{\text{exp}}$) of selected materials were taken from the reference article [1]. For the same materials, the simulated cross sections $\sigma_{\beta_{\text{sim}}}$ and the simulation uncertainty s_{sim} (reported as “simulated standard deviation” in the tables) were obtained from the Geant4 scoring results. The values of $\sigma_{\beta_{\text{sim}}}$ were computed using the same measurement geometry and the same cross-section definition as in the experiment.

The data were reported and analysed in three groups: elements, inorganic compounds, and organic compounds. The full experimental dataset is listed in Appendix A

3.6.2 Comparison metrics

This study considers how closely the Geant4 simulation reproduces the experimentally derived reflection cross sections σ_{β} . For each material, compared the experimental value with the simulated value is compared and quantified the agreement using three complementary metrics: relative deviation, z-score, and chi-square (χ^2). These metrics allow us to describe (i) the size of the difference, (ii) whether the difference is meaningful when uncertainties are considered, and (iii) the overall consistency across the full dataset [20].

For each material i , the dataset contains an experimental cross section $\sigma_{\beta_{\text{exp},i}} \pm s_{\text{exp},i}$ and a simulated cross section $\sigma_{\beta_{\text{sim},i}} \pm s_{\text{sim},i}$. The point-wise difference between simulation and experiment is defined as:

$$\Delta_i = \sigma_{\beta_{\text{sim},i}} - \sigma_{\beta_{\text{exp},i}} \quad (3.3)$$

The relative deviation(δ) was calculated according to Equation 3.4 to quantify the difference between the experimental and simulated results.

$$\delta_i(\%) = \frac{\Delta_i}{\sigma_{\beta_{\text{exp},i}}} \times 100\%. \quad (3.4)$$

To judge whether a difference is significant, uncertainties are considered from both experiment and simulation. Because the comparison is based on the difference Δ_i , its expected spread is determined by the combined uncertainty [21,22]:

$$s_i = \sqrt{s_{\text{exp},i}^2 + s_{\text{sim},i}^2}. \quad (3.5)$$

The z-score was then computed as:

$$z_i = \frac{\Delta_i}{s_i}. \quad (3.6)$$

The z-score indicates how many standard deviations separate the simulation from the experiment. As a practical interpretation, $|z_i| \leq 2$ was considered broadly consistent with the experimental result (within combined uncertainties), while larger values indicate increasing disagreement.

For each material, the chi-square contribution was calculated as shown in Eq. 3.7:

$$\chi_i^2 = \frac{\Delta_i^2}{s_i^2} = z_i^2. \quad (3.7)$$

This quantity is simply the square of the z-score ($\chi_i^2 = z_i^2$) and provides a standard way to accumulate agreement information across multiple data points. The total chi-square over a dataset was obtained by summing all contributions:

$$\chi^2 = \sum_i \chi_i^2. \quad (3.8)$$

A reduced chi-square was also reported to provide a reduced goodness-of-fit measure:

$$\chi_v^2 = \frac{\chi^2}{v}. \quad (3.9)$$

where v is the number of degrees of freedom [23]. Since no fitting parameters were introduced in this comparison, the number of degrees of freedom was taken as $v = N$ (the number of materials).

For the organic-compound dataset, simulated cross sections were systematically lower than the experimental values. Therefore, an additional analysis step was performed by introducing a scaling factor k applied to the simulated cross sections:

$$\sigma_{\beta_{s,i}} = k \sigma_{\beta_{\text{sim},i}} \quad (3.10)$$

The factor k was determined using a weighted minimum- χ^2 approach. First, a weighted chi-square function was defined as

$$\chi^2(k) = \sum_i w_i \left(k \sigma_{\beta_{\text{sim},i}} - \sigma_{\beta_{\text{exp},i}} \right)^2, \quad w_i = \frac{1}{s_{\text{exp},i}^2 + s_{\text{sim},i}^2} \quad (3.11)$$

The best scaling factor corresponds to the minimum of $\chi^2(k)$ and was obtained by setting the derivative with respect to k to zero $\left(\frac{d\chi^2}{dk} = 0 \right)$. This yields an analytical solution:

$$k = \frac{\sum_i w_i \sigma_{\beta_{\text{sim},i}} \sigma_{\beta_{\text{exp},i}}}{\sum_i w_i \sigma_{\beta_{\text{sim},i}}^2}. \quad (3.12)$$

After k was obtained, scaled simulated values were computed as $\sigma_{\beta_{s,i}} = k \sigma_{\beta_{\text{sim},i}}$. Since the scaling is multiplicative, the simulated uncertainties were scaled in the same way, $s_{s,i} = k s_{\text{sim},i}$. Agreement metrics (relative deviation, z -score, and chi-square contributions) were then recalculated using the updated combined uncertainty:

$$s'_{s,i} = \sqrt{s_{\text{exp},i}^2 + s_{s,i}^2} = \sqrt{s_{\text{exp},i}^2 + k^2 s_{\text{sim},i}^2} \quad (3.13)$$

Because this scaling introduces one fitted parameter, the degrees of freedom were taken as $\nu = N - 1$ for the scaled organic dataset, and results were reported after scaling.



4. RESULTS

The Geant4 simulation outputs ($\sigma_{\beta_{\text{sim}}}$) were compared against the experimental cross sections ($\sigma_{\beta_{\text{exp}}}$) for a total of 43 materials. The dataset was grouped into elements ($n = 13$), inorganic compounds ($n = 14$), and organic compounds ($n = 16$). Full numerical results (densities, molar mass, and cross sections) are provided in Appendix A.

For the elemental dataset ($N = 13$), Geant4-simulated cross sections $\sigma_{\beta_{\text{sim}}}$ were compared directly with the experimental values $\sigma_{\beta_{\text{exp}}} \pm s_{\text{exp}}$. No scaling or fitting parameters were introduced. The overall experimental–simulated agreement is shown in the parity plot in Figure 4.1, while the same comparison is also displayed as grouped bars with uncertainties in Figure 4.4. Closeness was reported using the relative deviation, while consistency including uncertainties was evaluated using the combined uncertainty to compute z -scores and chi-square. The total chi-square for this dataset was $\chi^2 = 87.53$. Since no fit parameters were used, the degrees of freedom were taken as $\nu = N = 13$, giving a reduced chi-square of $\chi^2_{\nu} = 6.73$. The material-wise z -scores are summarized in Figure 4.3. Several materials were consistent within combined uncertainties (Graphite, Nb, S, Mn, Pb; typically $|z| \lesssim 1$). In contrast, Fe and Cu were underestimated by the simulation ($z \approx -3$), while Sn was overestimated ($z \approx 2.9$). The chi-square breakdown is shown in Figure 4.2. The largest disagreement occurred for Ni ($z = -6.85$, $\chi^2_i = 46.86$), which contributed about half of the total χ^2 and largely drove the high χ^2_{ν} . Overall, the simulation shows reasonable agreement for several elements, but significant deviations remain for a subset of materials, most notably Ni (and also Fe and Cu).

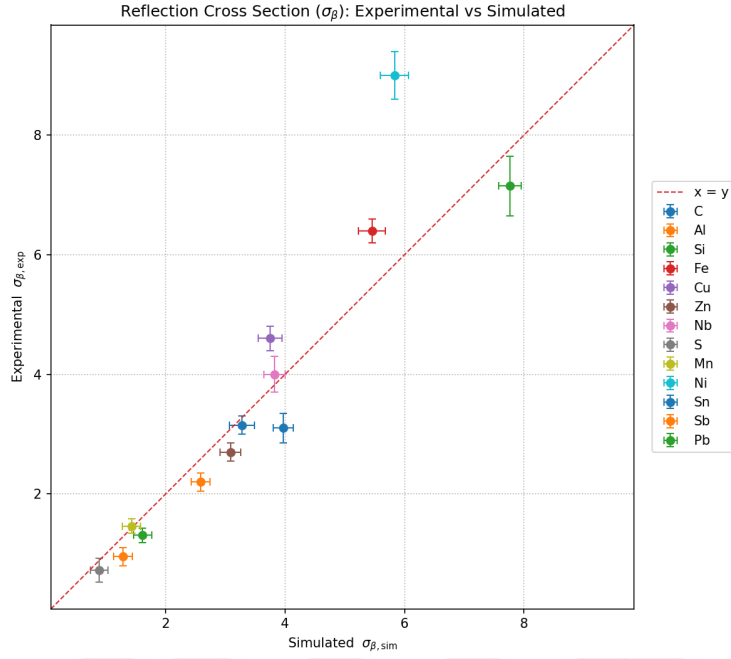


Figure 4.1: Experimental vs simulated reflection cross sections for the elemental dataset (with uncertainties). The dashed line indicates the $y = x$ reference.

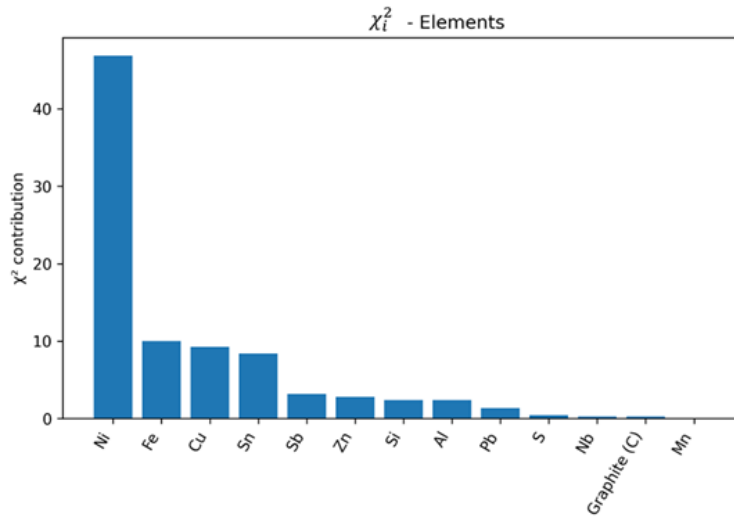


Figure 4.2: Individual chi-square contributions, χ_i^2 , for the elemental dataset.

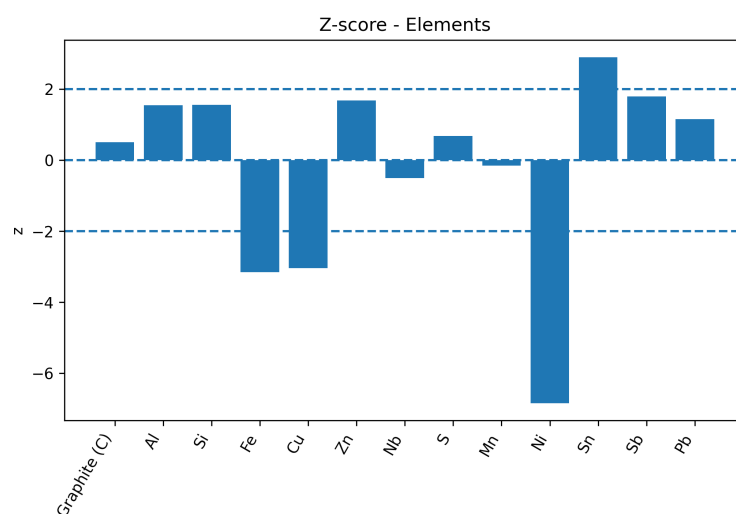


Figure 4.3: Standardized residuals (z-scores) for the elemental dataset. Dashed lines mark $z = \pm 2$.

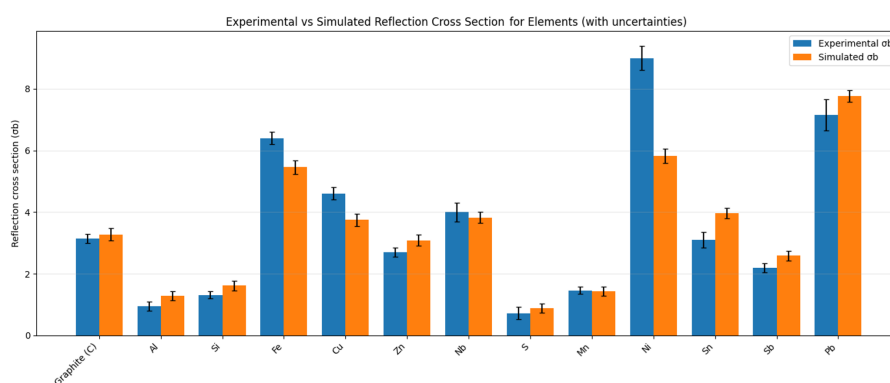


Figure 4.4: Experimental and simulated cross sections shown as grouped bars with uncertainties for the elemental dataset.

For the inorganic-compound subset ($N = 14$), Figure 4.5 compares the simulated and experimental effective reflection cross sections. Overall, the points lie close to the 1:1 line, suggesting that the simulation captures both the experimental scale and the relative ordering of the compounds within the quoted uncertainties. To quantify the agreement, an uncertainty-weighted chi-square was computed with no fitted parameters ($\nu = N = 13$), giving $\chi^2 = 37.74$ and a reduced value $\chi^2_\nu = 2.90$. This indicates that the spread between experiment and simulation is somewhat larger than what would be expected from the stated uncertainties, although most compounds remain compatible at the 2σ level. Figure 4.7 summarizes the point-by-point consistency using standardized residuals: 10 out of 13 compounds satisfy $|z| \leq 2$. Importantly, the discrepancy is not evenly shared across the dataset. As shown in Figure 4.6, the total χ^2 is dominated by ZrC ($\chi^2_i = 16.92$) and SrCO₃ ($\chi^2_i = 8.01$), which together contribute about 66% of the overall chi-square. The bar comparison in Figure 4.8 also makes the direction of these deviations clear. ZrC is systematically overestimated by the simulation (positive z), whereas SrCO₃ is underestimated (negative z). Aside from these outliers (and one borderline case near $|z| \approx 2$), the remaining compounds contribute only weakly to χ^2 and have z -scores close to zero, consistent with agreement within uncertainties. Al₂O₃ is included in the direct experimental-simulated bar comparison (see Figure 4.8); however, it is excluded from the uncertainty-weighted z -score and χ^2 statistics because no experimental uncertainty was available for this compound. Error bars indicate the reported experimental uncertainties and the Monte Carlo statistical uncertainties of the simulations.

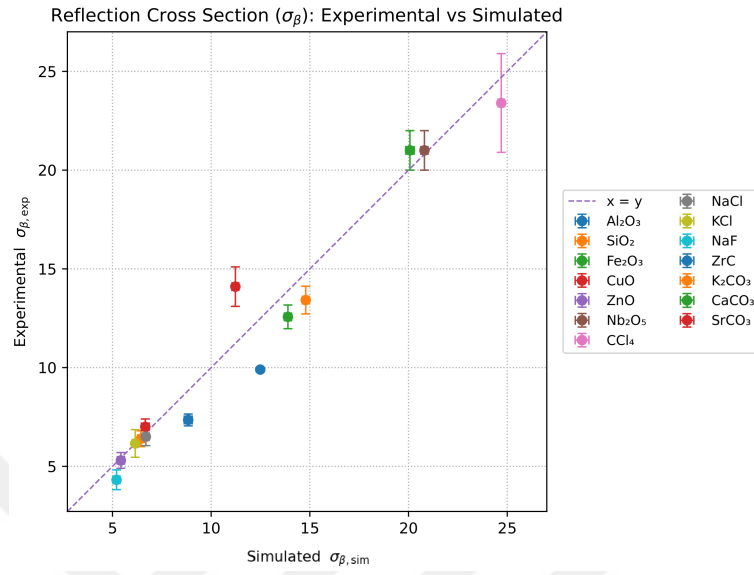


Figure 4.5: Experimental vs simulated reflection cross sections for the inorganic dataset (with uncertainties). The dashed line indicates the $y = x$ reference.

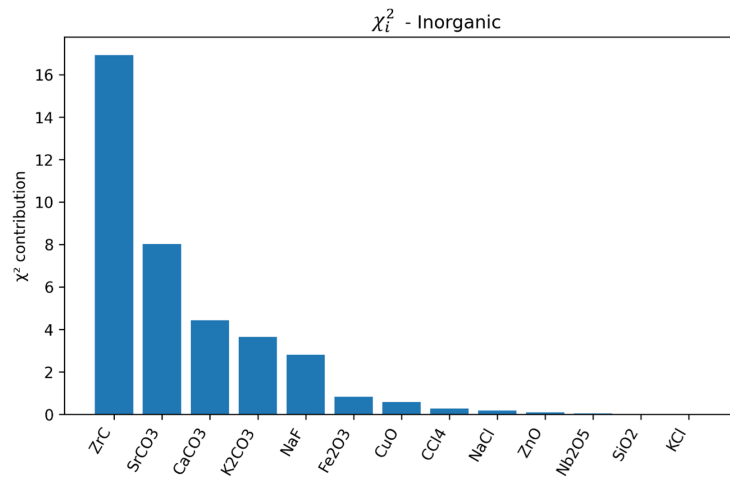


Figure 4.6: Individual chi-square contributions, χ_i^2 , for the inorganic dataset.

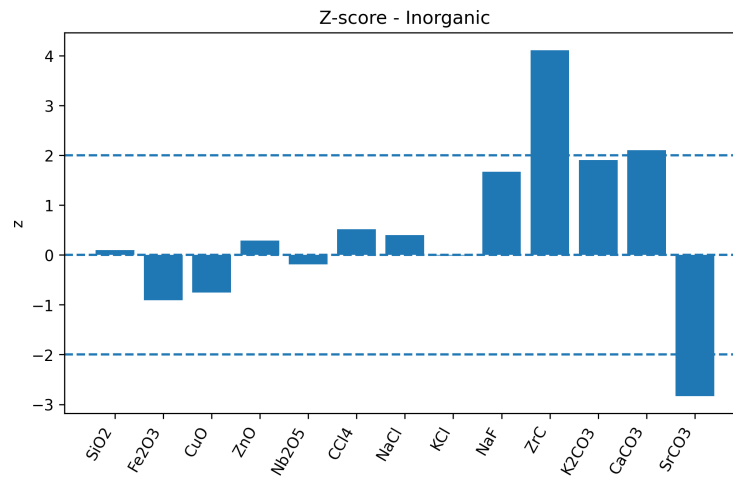


Figure 4.7: Standardized residuals (z -scores) for the inorganic dataset. Dashed lines mark $z = \pm 2$.

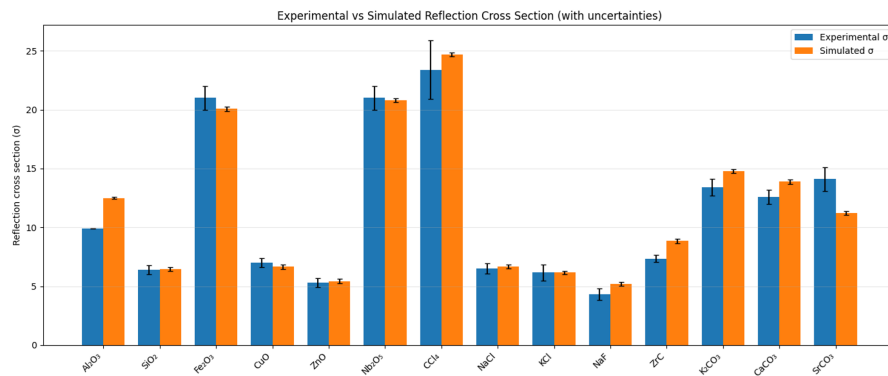


Figure 4.8: Experimental and simulated cross sections shown as grouped bars with uncertainties for the inorganic dataset.

For the organic-compound dataset ($N = 16$), Figure 4.9 shows that the simulated effective reflection cross sections are systematically lower than the experimental values for all materials, revealing a clear multiplicative (scale) bias. Before any scaling, the average relative deviation($\delta(\%)$) was $\approx -41.83\%$. To remove this global bias, a single scaling factor was applied to the simulated values, $k = 1.723 \pm 0.007$. After scaling, the data move close to the 1:1 line (Figure 4.9), and the average relative deviation($\delta(\%)$) decreases to 0.22% , showing that the main scale mismatch is largely corrected. Because one parameter was fitted, the number of degrees of freedom is $\nu = N - 1 = 15$. The uncertainty-weighted goodness-of-fit for the scaled dataset is $\chi^2 = 105.01$, corresponding to a reduced value $\chi^2_\nu = 7.00$. This indicates that, although the dominant multiplicative offset is removed, several material-specific discrepancies remain larger than expected from the combined uncertainties. The remaining tension is concentrated in a subset of compounds. Figures 4.10 and 4.11 show that the reduced χ^2 is dominated by a few large χ^2_i contributions and $|z| > 2$ outliers (notably acetone, butyl alcohol, benzene, benzyl alcohol, aniline, and diethyl ether), while most other organics have z -scores closer to zero. The bar comparison in Figure 4.12 provides the same message in absolute terms: after scaling, most pairs overlap within uncertainties, but a small number of compounds still deviate visibly, driving the large χ^2_ν .

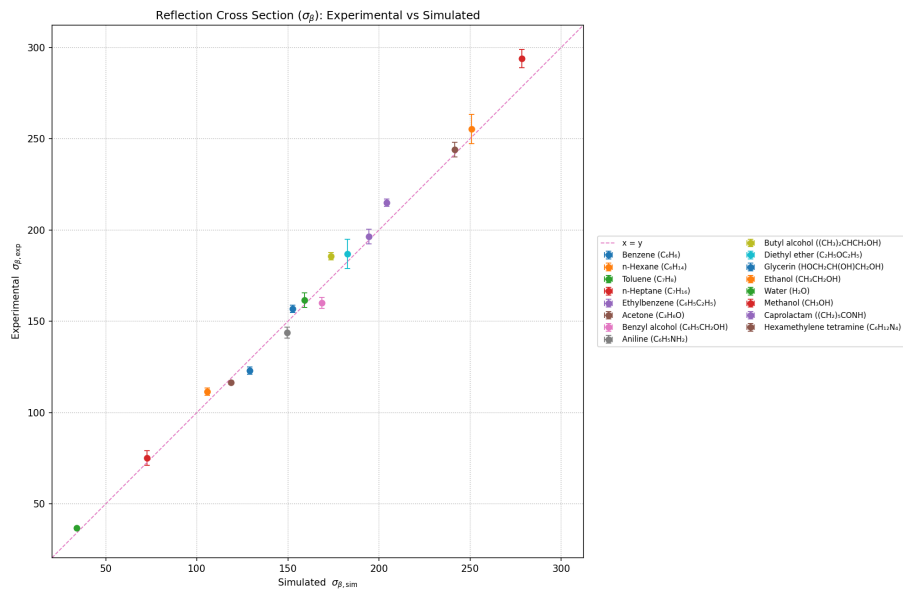


Figure 4.9: Experimental vs simulated reflection cross sections for the organic dataset (with uncertainties). The dashed line indicates the $y = x$ reference.

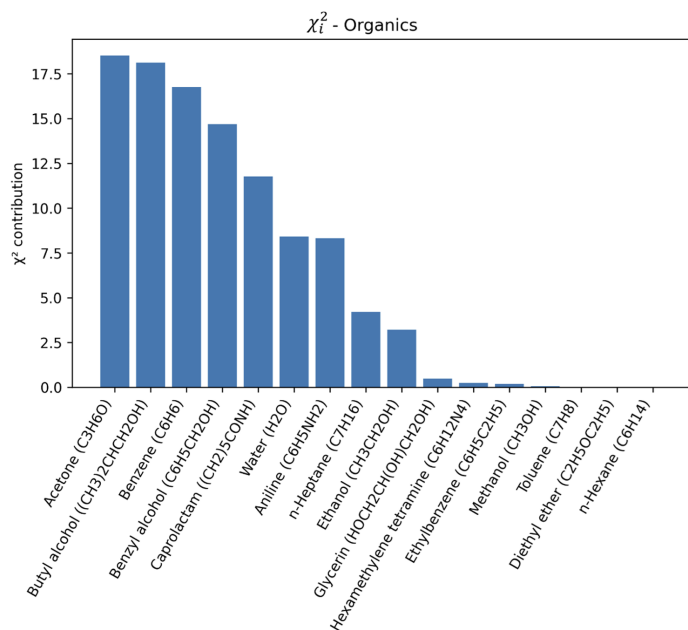


Figure 4.10: Chi-square contributions, χ_i^2 , for the organic-compound dataset after scaling.

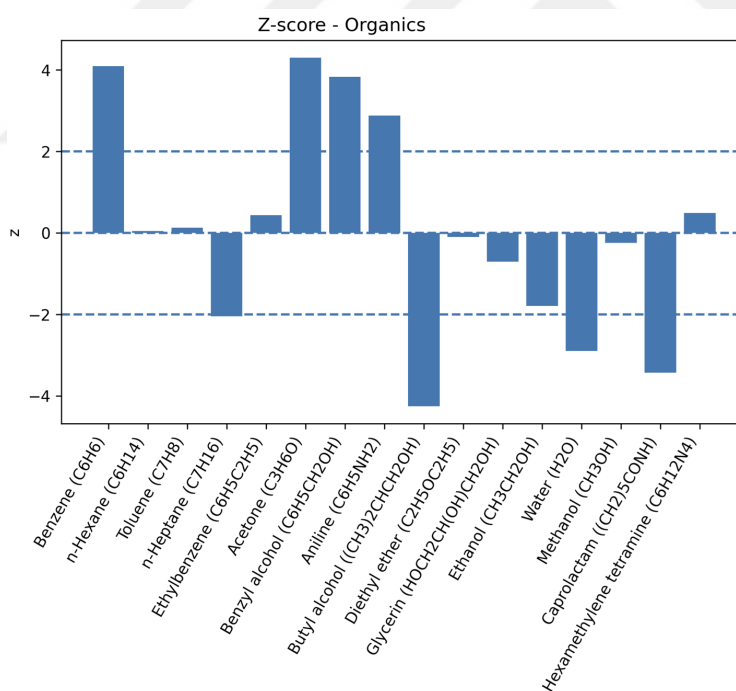


Figure 4.11: Standardized residuals (z -scores) for the organic dataset. Dashed lines mark $z = \pm 2$.

Figure 4.12 shows experimental and Geant4-simulated reflection cross sections for the selected organic materials. Error bars indicate the reported experimental uncertainties

and the Monte Carlo statistical uncertainties of the simulations. Correlation graph shows the organic compounds show a very strong positive correlation between the reflection cross section and the number of hydrogen atoms per molecule, consistent with the dominant role of hydrogen in low-energy neutron scattering(see Figure 4.13).

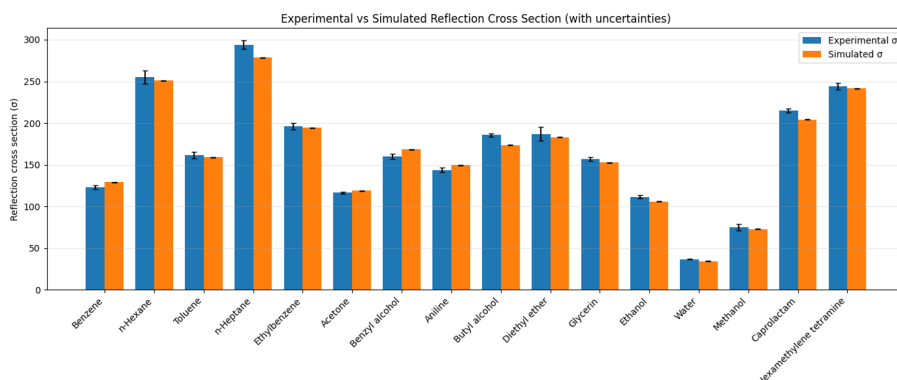


Figure 4.12: Bar graph of experimental and simulated reflection cross sections for organic compounds.

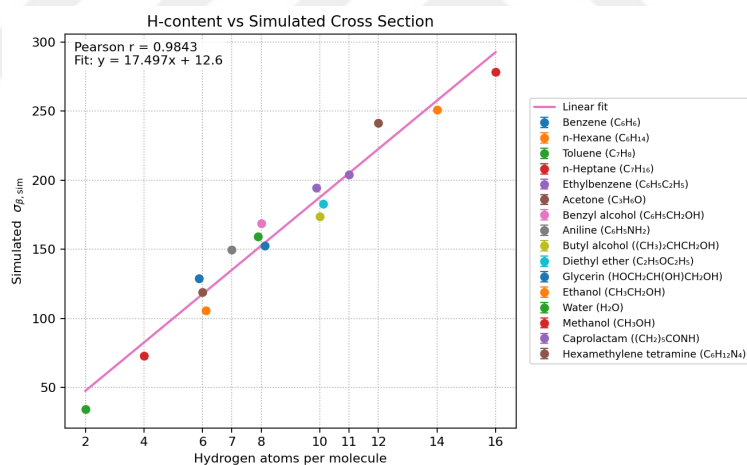


Figure 4.13: Correlation graph of reflection cross section and the number of hydrogen atoms per molecule($r=0.98$).



5. DISCUSSION

In this study, all materials were simulated with the same source-moderator-detector geometry, at the same sample position, and at the same sample thickness ($d = 1$ cm). The aim was thus to attribute the observed differences primarily to the material composition.

The comparison indicates two different behaviors across material classes. Elements and inorganic compounds largely follow the 1:1 trend, with a limited set of material-specific mismatches. In contrast, organic compounds show a coherent behavior: the simulated cross sections are lower than the experimental values across the whole group. Such a consistent shift is more consistent with a global scale bias than with isolated outliers.

In this work, the experimental detector response is represented by a scoring mesh placed between the moderator and the sample. Under this definition, the extracted “cross section” is an effective observable of the full setup. It depends on the neutron spectrum produced by moderator, transport through surrounding volumes, multiple scattering in the sample, and the probability that scattered neutrons enter the scoring region.

In high density materials, the practical consequence of this geometric sensitivity appears in the thickness dependence and saturation behavior. Csikai & Buczkó report that σ_β can remain nearly constant up to about 1 cm thickness for powder/liquid/solid samples; however, for high-density metals/alloys and strong absorbers, the $\sigma_\beta(d)$ relationship becomes nonlinear and tends toward saturation. For this reason, they state that they performed measurements using an approximately 2 mm layer and positioned the sample about 5 mm away from the moderator surface. Within this framework, the clear mismatches observed in our element set, especially for high-density metals (e.g., Ni, Fe, Cu), appear as an underestimation of the experimental σ_β values by the simulation.

However, the reference paper does not specify whether the samples were powders, liquids, or solids. As a result, the effective density and structure of the measured

samples are unclear, and the simulation, where materials are defined as homogeneous bulks, may not fully match the experimental sample conditions.

In organic compounds dataset, a single multiplicative scaling factor ($k=1.723\pm0.007$) strongly reduces the organic bias and brings the average scale into agreement. This supports the interpretation that the dominant difference for organics is a scale effect, not a random, material-by-material failure. Interestingly, increasing the sample radius for organic materials reduced the mismatch in a manner consistent with a simple rescaling of the simulation results, i.e., $\sigma_{\beta, sim}$ increased roughly by an approximately constant factor across organics.

This behaviour is consistent with an edge-leakage effect. In hydrogen-rich materials, small-radius samples can lose a fraction of the moderated/thermal neutrons laterally, whereas larger radii approach a semi-infinite response and increase the return probability. This pattern suggests that the organic bias may have a geometric component, in addition to material-related differences.

The literature reports that, the σ_{β} values attributed to hydrogen show a noticeable spread across different matrices, and it suggests that crystal-structure effects may contribute to thermal-neutron reflection cross sections. Therefore, differences in sample state may partly explain remaining experiment–simulation mismatches.

All simulations used 500,000 events. This is adequate to establish trends, but the scored observable is still count-based in a finite region and can be sensitive when the relevant contribution is a small fraction of transported neutrons. Increasing statistics and repeating a subset of materials is therefore a practical way to separate residual Monte Carlo variance from genuine systematic effects, especially for the few remaining outliers.

6. CONCLUSION AND RECOMMENDATIONS

This study compared experimental results with Geant4 simulations for effective reflection cross sections using the same Csikai–Buczkó geometry ($d = 1$ cm) [1]. For elements and inorganic compounds, the simulation agrees well with the experiment and follows an almost 1:1 trend, with only a few material-specific mismatches. For organic compounds, the simulation is consistently lower than the experimental values, suggesting a systematic scale bias. Applying one scaling factor ($k = 1.723 \pm 0.007$) largely corrects this organic shift, which means the main difference is systematic rather than random. Since the extracted value depends on the full setup, remaining differences may come from spectrum and geometry effects, sample size, or differences between the real sample state and the ideal material used in the simulation. Based on this findings and discussions presented above, the following recommendations are proposed:

- Increase Monte Carlo statistics for persistent mismatches.
Re-run the remaining outliers with more primary histories (e.g., 10^6 – 10^7) to check whether the deviations are due to limited statistics.
- Test sensitivity to physics models for low-energy neutrons.
Compare results using alternative hadronic settings to see how stable the response is in the moderator–sample–scoring region.
- Re-check material definitions against the experimental samples.
Verify assumptions on isotopic composition, density, and chemical state.
- Perform geometry sensitivity scans for finite-size and saturation effects.
Change sample radius (for organics) and sample thickness / distance to the moderator (for dense materials) and see how the mismatch changes.
- Check robustness against the scoring definition.
Repeat the extraction after small changes in the scoring-mesh position or size to quantify sensitivity to geometry.

These steps help separate class-wide scaling bias from material-specific discrepancies, and they strengthen the validation of Geant4 predictions versus the experimental effective observable.



REFERENCES

- [1] **Csikai, J. and Buczkó, C.M.** (1999). The concept of the reflection cross section of thermal neutrons, *Applied Radiation and Isotopes*, 50(3), 487–490.
- [2] **Csikai, J., Király, B. and Buczkó, C.M.** (2002). Targets for bulk hydrogen analysis using thermal neutrons, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 480(1), 166–170.
- [3] **Csikai, J. and ElAgib, I.** (1999). Bulk media assay using backscattered Pu–Be neutrons, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 432(2), 410–414.
- [4] **Csikai, J. and Dóczy, R.** (2007). A comparison of the neutron thermalization and reflection methods used for bulk hydrogen analysis, *Applied Radiation and Isotopes*, 65(7), 764–768.
- [5] **Lamarsh, J.R. and Baratta, A.J.** (2001). *Introduction to Nuclear Engineering*, Prentice Hall, Upper Saddle River, NJ, 3 edition, figure 3.4 (adapted).
- [6] **Knoll, G.F.** (2010). *Radiation Detection and Measurement*, John Wiley & Sons, Hoboken, NJ, 4th edition.
- [7] **Lewis, E.E.** (2008). *Fundamentals of Nuclear Reactor Physics*, Elsevier.
- [8] **Hussein, E.M.A.**, (2007). Chapter one—Mechanisms, **E.M.A. Hussein**, editor, *Radiation Mechanics*, Elsevier Science Ltd., pp.1–65.
- [9] **L'Annunziata, M.F.**, (2016). *Neutron Radiation, Radioactivity*, Elsevier, 2nd edition, pp.361–389.
- [10] **Jenkins, D.** (2020). *Radiation Detection for Nuclear Physics: Methods and Industrial Applications*, IOP Publishing, Bristol, UK.
- [11] **Mohapatra, D.K. and Reddy, C.P.** (2001). Use of neutron reflection method to assay nuclear materials in solutions, *Applied Radiation and Isotopes*, 55(5), 693–696.
- [12] **Csikai, J., El-Agib, I.M.A. and Buczkó, C.M.** (1998). Studies on the neutron reflection, scattering and transmission methods used for bulk hydrogen analysis, *Bulk Hydrogen Analysis Using Neutrons: Final Report of the 2nd Research Co-ordination Meeting*, International Atomic Energy Agency,

Vienna, research Co-ordination Meeting, Vienna, 17–20 Nov 1998; report no. IAEA/PS/RCM-98-2.

- [13] **Metropolis, N. and Ulam, S.** (1949). The Monte Carlo Method, *Journal of the American Statistical Association*, 44(247), 335–341.
- [14] **Carter, L.L. and Cashwell, E.D.** (1975). Particle-Transport Simulation with the Monte Carlo Method, **Technical report**, Los Alamos Scientific Laboratory.
- [15] **Agostinelli, S., Allison, J., Amako, K., Apostolakis, J., Araujo, H., Arce, P., Asai, M., Axen, D., Banerjee, S., Barrand, G. et al.** (2003). Geant4—A Simulation Toolkit, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 506(3), 250–303.
- [16] **Thomas, D.J., Kolkowski, P., Roberts, N.J., D’Mellow, B. and Joyce, M.J.** (2006). Investigation of a possible replacement for cadmium as a thermal neutron absorbing material in neutron instruments, **NPL Report DQL-RN 017**, National Physical Laboratory, Teddington, Middlesex, United Kingdom, <https://eprintspublications.npl.co.uk/id/eprint/3580>.
- [17] **Reyhancan, İ.A.** (1999). *Nötron spektrometresi ile tomografi ve hacimsel malzemelerin tahribatsız analizi*, Istanbul Technical University, Istanbul, Turkey, doctoral thesis (in Turkish). Database publication permission not granted; print copy available via university library (TÜBESS). 62 p. Advisor: H. Hüseyin Güven.
- [18] **Asai, M.** (2024). *Scoring I (Version 11.2-p01)*, Lecture slides, <https://indico.jlab.org/event/828/contributions/13967/attachments/10909/16532/Scoring1.pdf>, geant4 Tutorial Course, Jefferson Lab, Mar 26, 2024. Retrieved Feb 6, 2026.
- [19] **Allison, J., e.a.** (2016). Recent developments in Geant4, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 835, 186–225.
- [20] **Khair, U., Fahmi, H., Al Hakim, S. and Rahim, R.** (2017). Forecasting Error Calculation with Mean Absolute Deviation and Mean Absolute Percentage Error, *Journal of Physics: Conference Series*, volume930, p.012002, international Conference on Information and Communication Technology (IconICT), Medan, Sumatera Utara, Indonesia, 25–26 August 2017; published under licence by IOP Publishing Ltd.
- [21] **Joint Committee for Guides in Metrology** (2008). Evaluation of measurement data — Guide to the expression of uncertainty in measurement, **Technical Report JCGM 100:2008**, Joint Committee for Guides in Metrology (JCGM), <https://www.bipm.org/en/doi/10.59161/jcgm100-2008e>.

- [22] **Taylor, B.N. and Kuyatt, C.E.** (1994). Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results, **Technical Report 1297**, National Institute of Standards and Technology, <https://emtoolbox.nist.gov/publications/nisttechnicalnote1297s.pdf>, 1994 Edition; accessed 2026-02-01.
- [23] **Bevington, P.R. and Robinson, D.K.** (2003). *Data Reduction and Error Analysis for the Physical Sciences*, McGraw-Hill, New York, NY, 3 edition.





APPENDICES

APPENDIX A : Experimental Reflection Cross Sections and Simulated Reflection Cross Sections

APPENDIX B : Experimental Pu-Be Source Spectrum

APPENDIX C : Detector Construction-Key code snippets

APPENDIX D : Primary Generator Action -Key code snippets

APPENDIX E : Scoring Mesh Macro





Appendix A: Experimental Reflection Cross Sections and Simulated Reflection Cross Sections

Table A.1: Experimental reflection cross sections and simulated reflection cross sections for the elemental dataset.

Material	Density (g/cm ³)	Molar Mass (g/mol)	N (atoms/cm ³)	Experimental $\sigma_{\beta_{\text{exp}}} \pm \delta_{\text{exp}}$	R $(I - I_0)/I_0$	Simulated $\sigma_{\beta_{\text{sim}}}$	Simulated			Chi-sq (χ^2_i)
							Standard Deviation (s_{sim})	Relative Deviation(%)	$z - \text{score}$	
Graphite (C)	2.26	12.01	1.13E+23	3,15 ± 0,15	0.37	3.27	0.20	4,02	0,50	0,246
Al	2.70	26.98	6.03E+22	0,95 ± 0,15	0.077	1.28	0.15	34,96	1,54	2,378
Si	2.33	28.09	5.00E+22	1,31 ± 0,12	0.08	1.61	0.15	23,20	1,55	2,395
Fe	7.87	55.85	8.49E+22	6,40 ± 0,20	0.46	5.45	0.22	-14,77	-3,16	9,995
Cu	8.96	63.55	8.49E+22	4,6 ± 0,2	0.31	3.74	0.19	-18,50	-3,04	9,248
Zn	7.14	65.38	6.57E+22	2,7 ± 0,15	0.20	3.08	0.17	14,26	1,67	2,796
Nb	8.57	92.91	5.56E+22	4,0 ± 0,30	0.21	3.82	0.17	-4,39	-0,50	0,254
S	2.07	32.06	3.89E+22	0,72 ± 0,20	0.03	0.88	0.14	23,28	0,67	0,454
Mn	7.21	54.94	7.90E+22	1,46 ± 0,12	0.11	1.42	0.15	-2,17	-0,16	0,026
Ni	8.90	58.69	9.13E+22	9,0 ± 0,40	0.53	5.83	0.23	-35,19	-6,85	46,861
Sn	7.31	118.71	3.71E+22	3,10 ± 0,25	0.14	3.96	0.16	28,04	2,89	8,368
Sb	6.68	121.76	3.30E+22	2,20 ± 0,15	0.08	2.58	0.15	17,46	1,78	3,184
Pb	11.34	207.20	3.29E+22	7,15 ± 0,5	0.25	7.76	0.18	8,58	1,15	1,319

Table A.2: Experimental reflection cross sections and simulated reflection cross sections for the inorganic-compound subset.

Material	Density (g/cm ³)	Molar Mass (g/mol)	N (atoms/cm ³)	Experimental $\sigma_{\beta_{\text{exp}}} \pm s_{\text{exp}}$	R $(I - I_0)/I_0$	Simulated			Relative Deviation (%)	$z - score$	Chi-sq (χ_i^2)
						Simulated $\sigma_{\beta_{\text{sim}}}$	Standard Deviation (s_{sim})	Deviation			
Al ₂ O ₃	3.95	101.96	2.33296E+22	9,9	0,29	12,48	0,08	26,14	–	–	–
SiO ₂	2.65	60.08	2.65618E+22	6,4 ± 0,4	0,17	6,44	0,17	0,68	0,10	0,010	0,010
Fe ₂ O ₃	5.24	159.69	1.97603E+22	21,0 ± 1,0	0,39	20,07	0,21	-4,42	-0,91	0,825	0,825
CuO	6.31	79.55	4.77672E+22	7,0 ± 0,4	0,31	6,66	0,19	-4,80	-0,75	0,569	0,569
ZnO	5.61	81.38	4.15132E+22	5,3 ± 0,4	0,22	5,42	0,18	2,39	0,29	0,083	0,083
Nb ₂ O ₅	4.60	265.81	1.04214E+22	21,0 ± 1,0	0,21	20,80	0,18	-0,93	-0,19	0,037	0,037
CCl ₄	1.59	153.82	6.22480E+21	23,4 ± 2,5	0,15	24,69	0,16	5,54	0,52	0,268	0,268
NaCl	2.16	58.44	2.22579E+22	6,5 ± 0,45	0,14	6,69	0,16	2,96	0,40	0,160	0,160
KCl	1.98	74.55	1.59940E+22	6,16 ± 0,7	0,09	6,15	0,16	-0,12	-0,01	0,000	0,000
NaF	2.56	41.99	3.67143E+22	4,32 ± 0,50	0,19	5,20	0,17	20,52	1,67	2,797	2,797
ZrC	6.59	103.24	3.84395E+22	7,35 ± 0,30	0,33	8,83	0,20	20,24	4,11	16,920	16,920
K ₂ CO ₃	2.43	138.21	1.05878E+22	13,42 ± 0,7	0,15	14,79	0,16	10,22	1,91	3,630	3,630
CaCO ₃	2.71	100.09	1.63049E+22	12,57 ± 0,6	0,22	13,88	0,18	10,50	2,10	4,426	4,426
SrCO ₃	3.70	147.63	1.50927E+22	14,10 ± 1,0	0,16	11,22	0,17	-20,37	-2,83	8,012	8,012

Table A.3: Experimental reflection cross sections and simulated reflection cross sections for the organic-compound subset.

Material	Density (g/cm ³)	Molar Mass (g/mol)	N (atoms/cm ³)	Experimental $\sigma_{\beta_{\text{exp}}} \pm \delta_{\text{exp}}$	R $(I - I_0)/I_0$	Simulated			Relative Deviation (%)	$z - \text{score}$	Chi-sq (χ^2_t)
						Simulated $\sigma_{\beta_{\text{sim}}}$	Standard Deviation (s_{sim})				
Benzene (C ₆ H ₆)	0.879	78.11	6.77677E+21	123,0 ± 2	0.51	128,95	0,39		4,84	2,92	8,524
n-Hexane (C ₆ H ₁₄)	0.660	86.18	4.61188E+21	255,3 ± 8	0.68	250,98	0,43		-1,69	-0,54	0,291
Toluene (C ₇ H ₈)	0.867	92.14	5.66646E+21	161,5 ± 4	0.53	159,03	0,41		-1,53	-0,61	0,377
n-Heptane (C ₇ H ₁₆)	0.684	100.20	4.11083E+21	293,9 ± 5	0.67	278,42	0,43		-5,27	-3,08	9,513
Ethylbenzene (C ₆ H ₅ C ₂ H ₅)	0.867	106.17	4.91765E+21	196,4 ± 4	0.56	194,50	0,41		-0,96	-0,47	0,221
Acetone (C ₃ H ₆ O)	0.784	58.08	8.12887E+21	116,4 ± 1	0.57	118,83	0,411		2,09	2,06	4,239
Benzyl alcohol (C ₆ H ₅ CH ₂ OH)	1.045	108.14	5.81930E+21	160,1 ± 3	0.57	168,56	0,41		5,29	2,80	7,814
Aniline (C ₆ H ₅ NH ₂)	1.021	93.13	6.60202E+21	143,7 ± 3	0.58	149,65	0,415		4,14	1,36	1,841
Butyl alcohol ((CH ₃) ₂ CHCH ₂ OH)	0.810	74.12	6.58098E+21	185,6 ± 2	0.67	173,63	0,44		-6,45	-5,84	34,086
Diethyl ether (C ₂ H ₅ OC ₂ H ₅)	0.713	74.12	5.79288E+21	187,0 ± 8	0.62	182,77	0,42		-2,26	-0,53	0,279
Glycerin (HOCH ₂ CH(OH)CH ₂ OH)	1.260	92.09	8.23946E+21	156,8 ± 2	0.74	152,53	0,45		-2,72	-1,18	1,401
Ethanol (CH ₃ CH ₂ OH)	0.789	46.07	1.03133E+22	111,5 ± 2	0.64	105,83	0,43		-5,07	-2,76	7,620
Water (H ₂ O)	1.000	18.02	3.34184E+22	36,8 ± 0,5	0.67	34,20	0,440		-7,03	-3,88	15,073
Methanol (CH ₃ OH)	0.791	32.04	1.48670E+22	75,1 ± 4	0.63	72,76	0,42		-3,10	-0,58	0,334
Caprolactam ((CH ₂) ₅ CONH)	1.010	113.16	5.37489E+21	215,0 ± 2	0.64	204,13	0,43		-5,04	-5,29	27,976
Hexamethylene tetramine (C ₆ H ₁₂ N ₄)	1.330	140.19	5.71315E+21	244,0 ± 4	0.81	241,47	0,47		-1,03	-0,63	0,397



Appendix B: Experimental Pu-Be Source Spectrum

Table B.1: Discrete neutron-energy grid with relative weights, normalized weights, and cumulative probability.

Index	Neutron energy E_i (MeV)	Relative weight (w_i)	Normalized weight ($w_i / \sum w_i$)	Cumulative probability $F(E_i)$
1	0.00	0.0000	0.000000	0.000000
2	0.25	0.0600	0.020219	0.020219
3	0.50	0.0450	0.015164	0.035383
4	0.70	0.0550	0.018534	0.053917
5	1.00	0.0450	0.015164	0.069082
6	1.40	0.0500	0.016849	0.085931
7	1.75	0.0400	0.013479	0.099410
8	2.00	0.0550	0.018534	0.117944
9	2.50	0.0900	0.030329	0.148273
10	2.75	0.1550	0.052233	0.200505
11	3.00	0.2200	0.074137	0.274642
12	3.10	0.2400	0.080877	0.355519
13	3.25	0.2050	0.069081	0.424600
14	3.50	0.1900	0.064027	0.488627
15	4.00	0.1850	0.062343	0.550970
16	4.50	0.1950	0.065711	0.616681
17	4.75	0.1900	0.064027	0.680708
18	5.00	0.1700	0.057277	0.737985
19	5.50	0.1300	0.043807	0.781792
20	6.00	0.0200	0.006740	0.788532
21	6.50	0.1150	0.038752	0.827284
22	7.00	0.0700	0.023589	0.850873
23	7.75	0.1100	0.037067	0.887940
24	8.00	0.1000	0.033699	0.921639
25	8.50	0.0500	0.016849	0.938488
26	9.00	0.0200	0.006740	0.945228
27	9.50	0.0350	0.011794	0.957022
28	9.75	0.0500	0.016849	0.973884
29	10.00	0.0400	0.013479	0.987363
30	10.25	0.0300	0.010110	0.997473
31	10.50	0.0075	0.002527	1.000000
32	10.75	0.0000	0.000000	1.000000



Appendix C: Geant4 DetectorConstruction.cc Code Snippets

```
G4VPhysicalVolume* DetectorConstruction::ConstructVolumes()
{
    G4GeometryManager::GetInstance()->OpenGeometry();
    G4PhysicalVolumeStore::GetInstance()->Clean();
    G4LogicalVolumeStore::GetInstance()->Clean();
    G4SolidStore::GetInstance()->Clean();

    G4NistManager* nist = G4NistManager::Instance();

    // Material definitions
    G4Element* elO = new G4Element("Oxygen", "O", 8.,
    16.00*g/mole);
    G4Element* elH = nist->FindOrBuildElement("H");
    G4Element* elC = nist->FindOrBuildElement("C");
    G4Element* elN = nist->FindOrBuildElement("N");
    G4Element* elF = nist->FindOrBuildElement("F");
    G4Material* cadmium = nist->FindOrBuildMaterial("G4_Cd");

    // CH2 (Polyethylene) moderator
    G4Material* matCH2 = new G4Material("Polyethylene",
    0.94*g/cm3, 2);
    matCH2->AddElement(elC, 85.63*perCent);
    matCH2->AddElement(elH, 14.37*perCent);

    // Example organic sample material: Methanol CH4O
    G4Material* Methanol = new G4Material("Methanol",
    0.7918*g/cm3, 3);
    Methanol->AddElement(elC, 37.48*perCent);
    Methanol->AddElement(elH, 12.58*perCent);
    Methanol->AddElement(elO, 49.94*perCent);

    // Enriched boron for BF3: 96% B-10, 4% B-11
    G4Isotope* isoB10 = new G4Isotope("B10", 5, 10,
    10.0129370*g/mole);
    G4Isotope* isoB11 = new G4Isotope("B11", 5, 11,
    11.0093055*g/mole);

    G4Element* elB_enriched =
    new G4Element("Enriched Boron", "B", 2);
    elB_enriched->AddIsotope(isoB10, 96.*perCent);
    elB_enriched->AddIsotope(isoB11, 4.*perCent);

    // BF3 gas
    G4double density = 2.42*mg/cm3;
    G4Material* matBF3 = new G4Material("BF3_Gas",
    density, 2, kStateGas);
    matBF3->AddElement(elB_enriched, 1);
    matBF3->AddElement(elF, 3);
    //....
```

```

// Sample
G4ThreeVector position(0, 11.15*cm, 0);
G4RotationMatrix* yRot = new G4RotationMatrix;
yRot->rotateX(90.*deg);

G4double spRMin = 0.*cm;
G4double spRMax = 5.1*cm;
G4double spDz   = 0.5*cm;
G4double spSPhi = 0.*deg;
G4double spDPhi = 360.*deg;

auto sample = new G4Tubs("sample", spRMin,
spRMax, spDz, spSPhi, spDPhi);

auto sampleL = new G4LogicalVolume(sample,
Methanol, "Sample");
new G4PVPlacement(yRot,
                  position,
                  sampleL,
                  "sample",
                  lWorld,
                  false,
                  0,
                  true);

// Cd geometry (open-top box)
G4double t = 0.05*cm;

G4double pX = 4.1*cm;
G4double pY = 1.25*cm;
G4double pZ = 1.25*cm;

auto cadmiums = new G4Box("cadm", pX, pY, pZ);

G4double spX = pX - t;
G4double spY = pY - t;
G4double spZ = pZ;

auto subcad = new G4Box("subcad", spX, spY, spZ);

auto cadsub =
new G4SubtractionSolid("CdOpenTopBox",
                      cadmium,
                      subcad,
                      nullptr,
                      G4ThreeVector(0, 0, +t));

auto logicShape4 =
new G4LogicalVolume(cadsub, G4Cd, "Shape4");

new G4PVPlacement(yRot, G4ThreeVector(0, 8.5*cm, 0),
logicShape4, "Shape4", lWorld, false, 0, true);
return fPWorld;
}

```

Appendix D: Geant4 PrimaryGeneratorAction.cc Code Snippets

```
void PrimaryGeneratorAction::BuildPuBeSpectrumCDF()
{
    std::vector<std::pair<G4double,G4double>> raw = {
        {0.0*MeV, 0.0}, {0.25*MeV, 0.06}, {0.5*MeV, 0.045},
        /* ... (all nodes; see Appendix B for full table) ... */
        {10.5*MeV, 0.0075}, {10.75*MeV, 0.0}
    };

    G4double sum = 0.0;
    for (const auto& p : raw) sum += p.second;

    G4double cum = 0.0;
    fSpectrum.clear();
    for (const auto& p : raw) {
        cum += p.second / sum;
        fSpectrum.emplace_back(p.first, cum); // (E, CDF)
    }
}

G4double PrimaryGeneratorAction::SamplePuBeEnergy()
{
    const G4double r = fUniDist(fRng); // U[0,1)
    auto it = std::lower_bound(
        fSpectrum.begin(), fSpectrum.end(), r,
        [](const auto& entry, G4double value){ return entry.second < value; }
    );
    if (it == fSpectrum.end()) --it;
    return it->first;
}
```



Appendix E: Geant4 Scoring Mesh Macro: Key Snippets

```
# --- Scoring mesh (detector-region virtual counter) ---
/score/create/boxMesh ThermalMesh
/score/mesh/boxSize 5.2 0.2 5.2 cm
/score/mesh/nBin 1 1 1
/score/mesh/translate/xyz 0. 10.63 0. cm
# --- Quantity: track count proxy in the mesh volume ---
/score/quantity/volumeFlux Npass
# --- Thermal-neutron selection---
/score/filter/particleWithKineticEnergy nTh1 0. 5e-7 MeV neutron
/score/close
/score/list
```



CURRICULUM VITAE

NAME SURNAME: Zehra GÜZEL

EDUCATION:

- **B.Sc.:** 2023, Istanbul Technical University, Science and Letter Faculty, Physics Engineering Department

PROFESSIONAL EXPERIENCE AND REWARDS:

- 2022 Internship, Istanbul Technical University, Physics Engineering Department
- 2022 Internship, Turkish Energy, Nuclear and Mineral Research Agency (TENMAK)
- 2025-Present Researcher, BEAMIDE S.r.l.

