Efficient Monte Carlo framework for evaluating thermal and epithermal neutron self-shielding in electron-beam-driven neutron activation analysis

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Date: 2025-07-23T00:00:00+00:00

Abstract

Neutron self-shielding factors play a crucial role in accurately interpreting neutron activation analysis by accounting for neutron flux attenuation within specimens, however calculating these factors in complex systems is computationally intensive and time-consuming. This study introduces a two-stage "sequence-calculation" framework that significantly enhances the efficiency of Monte Carlo simulations for neutron self-shielding analysis, particularly when one needs to consider multiple specimens and irradiation positions. The proposed method is validated through a cross-code validation using the Particle and Heavy Ion Transport Code System (PHITS) and Monte Carlo N-Particle Transport Code version 6 (MCNP6), both of which express a reasonable agreement with the conventional Monte Carlo method. The method was applied to evaluate thermal and epithermal neutron self-shielding factors for Au, Cu, W, and Zr activation specimens, which are irradiated using the Intense Resonance Neutron Source (IREN) at the Joint Institute for Nuclear Research (JINR), Dubna. These values are fundamental for upcoming researches with IREN. Thanks to the significant reduction in computational time enabled by the proposed approach, the study is able to explore the sensitivity of self-shielding effect to specimen thickness and neutron flux variation, emphasizing the need for geometry-specific corrections. Beyond the neutron self-shielding problem, the proposed framework offers a robust and versatile solution for a wide range of radiation transport problems involving complex geometries and source terms.

Full Text

Preamble

Efficient Monte Carlo Framework for Evaluating Thermal and Epithermal Neutron Self-Shielding in Electron-Beam-Driven Neutron Activation Analysis

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Neutron self-shielding factors play a crucial role in accurately interpreting neutron activation analysis by accounting for neutron flux attenuation within specimens. However, calculating these factors in complex systems is computationally intensive and time-consuming. This study introduces a two-stage "sequence-calculation" framework that significantly enhances the efficiency of Monte Carlo simulations for neutron self-shielding analysis, particularly when multiple specimens and irradiation positions must be considered. The proposed method is validated through cross-code comparison using the Particle and Heavy Ion Transport Code System (PHITS) and Monte Carlo N-Particle Transport Code version 6 (MCNP6), both of which show reasonable agreement with conventional Monte Carlo methods. The method was applied to evaluate thermal and epithermal neutron self-shielding factors for Au, Cu, W, and Zr activation specimens irradiated using the Intense Resonance Neutron Source (IREN) at the Joint Institute for Nuclear Research (JINR), Dubna. These values are fundamental for upcoming research with IREN. Thanks to the significant reduction in computational time enabled by the proposed approach, the study explores the sensitivity of self-shielding effects to specimen thickness and neutron flux variation, emphasizing the need for geometry-specific corrections. Beyond the neutron self-shielding problem, the proposed framework offers a robust and versatile solution for a

wide range of radiation transport problems involving complex geometries and source terms.

Keywords: Monte Carlo simulation, electron-beam-driven neutron source, sequence-calculation framework, thermal neutron self-shielding, epithermal neutron self-shielding

Introduction

To accurately interpret neutron activation measurements, neutron self-shielding correction factors—commonly referred to as g-factors—are introduced to account for deviations of the neutron spectrum inside the activation specimen from that at its surface. These distortions arise because neutrons are scattered and absorbed as they penetrate the material. The g-factors depend significantly on several parameters, including the direction and energy distribution of the neutron field, as well as the nuclear reaction cross-section, mass density, and geometric configuration of the specimen. Due to their sensitivity to these variables, g-factors often need to be recalculated for each specific experimental setup. Given their critical role in ensuring the accuracy of activation analysis and the frequency with which they must be determined, it is essential to develop a method for calculating g-factors that is both computationally efficient and robust in delivering accurate results.

Monte Carlo (MC) simulations are often employed to determine g-factors thanks to their effectiveness in resolving energy-dependent cross-sections and complex geometric details, despite their high computational cost and cumbersomeness. Several MC-based studies on g-factors in various neutron facilities are listed in Table 1, illustrating the widespread reliance on this method. The MC-based method is particularly effective when neutron source characteristics are well-defined and relatively simple. For instance, they perform well in scenarios involving isotropic neutron emission from radioactive sources such as Am-Be, spontaneous fission ^{252}Cf, and Pu-Be, where both spatial and energy distributions are predictable. However, in more complex situations where neutrons are indirectly generated, the application of MC simulations becomes significantly more challenging due to increased computational demands. A typical example is neutron production via the bombardment of charged particles on thick targets, where the resulting neutron field often exhibits complex, anisotropic spatial distributions and broad, poorly defined energy spectra. These conditions require more detailed modeling and longer simulation times, limiting the practicality of MC methods for routine or time-sensitive evaluations.

In recent years, accelerator-driven neutron sources have gained popularity for neutron experiments due to advantages such as lower cost, instant ON/OFF control, tunable beam parameters, and enhanced safety compared to reactor-based sources. The Intense Resonance Neutron Source (IREN) at the Joint Institute for Nuclear Research (JINR) in Dubna, Russia has been employed by our group for nuclear data measurements using the neutron activation technique. In our

experiments, activation specimens are placed outside the moderator tank and irradiated by neutrons streaming from the moderator, resulting in an anisotropic neutron field. Under such conditions, analytical methods based on isotropic assumptions are no longer valid.

The present work aims to advance the application of MC-based methods for evaluating g-factors in complex neutron fields. To address the challenge of high computational demands, a delicate calculation strategy is proposed to enhance the efficiency of MC simulations while preserving their accuracy. This approach has been applied to determine the thermal and epithermal neutron self-shielding factors, denoted as G and G respectively, for activation experiments using the IREN facility. The remainder of this article is organized as follows. Section II provides a detailed description of the system configuration and introduces the proposed MC calculation strategy for determining G and G . Section III discusses the effectiveness and accuracy of the method, with particular attention to the dependence of g-factors on the angular distribution of the neutron field. Conclusions are given in the final section.

II. Description of Investigated System and Monte Carlo Strategy

A. Investigated System

The configuration of the electron-beam-driven neutron source, namely IREN, employed in this study is illustrated in Fig. 1. The core component of the IREN facility is a linear electron accelerator (LUE-200) capable of accelerating electrons to a maximum energy of 200 MeV. The parameters of the LUE-200 accelerator used in this study are listed in Table 2. High-energy electrons with pencil-beam geometry (30 mm in diameter) from the LUE-200 accelerator irradiate a water-filled aluminum converter under vacuum conditions.

The beam is first focused by a hemispherical-shell titanium (Ti) lens (0.4 mm thick, 18 mm diameter) mounted centrally at the converter' s front face, then impinges on a cylindrical tungsten-dominated target (100 mm length, 40 mm diameter) aligned along the converter' s central axis. The target, with a composition of 90% tungsten (W), 3% iron (Fe), and 7% nickel (Ni) by mass, exhibits an effective density of 18.23 g/cm^3 based on its stoichiometry. The target is embedded within a moderator composed of a cylindrical aluminum container (converter' s case) (205 mm length, 160 mm diameter) filled with distilled water for neutron thermalization. Neutrons produced via the (e, γ) and (γ, n) nuclear reactions within the target are thermalized within this moderator. The water is circulated by a pump to remove heat from the target.

Four natural high chemical-purity (>99.99%) specimens—including gold (Au), copper (Cu), W, and zirconium (Zr)—are considered in the present work because their relevant g-factors are required for upcoming research at IREN, where the absorption cross-sections and resonance integrals of some selected isotopes of

Cu, W, and Zr will be measured relative to those of Au. The specimen in the form of a rectangular thin foil is positioned along the converter such that its planar surfaces interface directly with the converter's sidewall. The isotopic composition of the foils follows natural abundance, whereas the associated nuclear reaction cross-sections are taken from validated libraries, namely JENDL-4.0 and ENDF/B-VII.1. Specific values of geometric and material parameters for both the converter and specimens are summarized in Table 3.

B. Monte Carlo Simulations and the Proposed "Sequence-Calculation" Framework

The g-factor is defined as the ratio of the reaction rate in the actual specimen to that in an infinitely diluted one:

$$g = \frac{\int_{E_1}^{E_2} \phi(E)\sigma_\gamma(E)dE}{\int_{E_1}^{E_2} \phi_0(E)\sigma_\gamma(E)dE}$$

where $\phi(E)$ and $\phi_0(E)$ are the neutron flux energy distributions in the actual and infinitely diluted specimens, respectively, while $\sigma_\gamma(E)$ is the (n, γ) cross-section of the investigated isotope, which can be taken from nuclear reaction databases such as ENDF/B-VII.1 and JENDL-4.0. The integration bounds E_1 and E_2 are defined as $E_1 = 10^{-3}$ eV and $E_2 = 0.5$ eV for G_{th}, and $E_1 = 0.5$ eV and $E_2 = 0.2$ MeV for G_{epi}. Accurate determination of $\phi(E)$ and $\phi_0(E)$ is therefore central to reliable calculation of g-factors.

In the present study, $\phi(E)$ and $\phi_0(E)$ are obtained from MC simulations, which were mostly performed using the Particle and Heavy Ion Transport Code System (PHITS v3.21). Some selected configurations were also computed using the Monte Carlo N-Particle Transport Code version 6 (MCNP6) for cross-validation. Unless otherwise specified, all simulation results presented hereafter were obtained using PHITS. To approximate the infinitely diluted condition, a zero-density (void) tally with identical dimensions to the corresponding specimen was implemented in the simulation. This void tally effectively excludes self-shielding interactions, providing the unperturbed neutron flux reference. The MC simulation parameters for PHITS and MCNP6 are summarized in Table 4. In PHITS, neutron fluxes in the specimen' s volume and surface are quantified via the T-Track and T-Cross tallies, respectively. For MCNP6, only volumetric flux was computed using the F4 tally. Angular and energy distributions of the neutron flux were resolved using angle and energy meshes, respectively. G_{th} and G_{epi} were computed by adopting the 640-group energy structure from the MATSSF database, which is specifically recommended for neutron activation analysis (NAA) applications. Within this structure, cross-section values for each energy group were derived by averaging $\sigma_\gamma(E)$ over the group' s energy interval.

Conventional MC simulations for estimating neutron fluxes $\phi(E)$ and $\phi_0(E)$ often require substantial computational time due to two key challenges: (1) the complexity of electron- and photon-induced nuclear reactions in neutron production from electron beam-converter interactions, and (2) the low geometric efficiency of neutron detection in cm^3-scale specimens, where most neutrons fail to intersect the region of interest. Since g-factors vary depending on the specific specimen under investigation, using conventional MC simulations to calculate g-factors for many specimens becomes impractical. For instance, simulating a single experimental configuration with our setup can take over a month on a typical personal computer (PC) and nearly one week on a powerful workstation.

To facilitate efficient determination of g-factors across diverse specimens, we propose a "sequence-calculation" framework, whose schematic workflow is shown in Fig. 2. In this framework, we separate the whole simulation into two parts, represented by Program-1 and Program-2. Program-1 simulates neutron generation from electron beam-converter interactions, recording transport data including particle type, coordinate, directional vector, flux, energy, and statistical history of all neutrons crossing a defined "surface source." The latter is a subsection of the converter's sidewall encompassing the specimen irradiation area.

It is worth noting that PHITS is capable of recording transport data not only for neutrons but also for electrons and photons crossing the defined surface source. However, in our study, only neutrons were recorded, as the contributions of electrons and photons to Program-2 results were found to be negligible, while their inclusion significantly increased computational time (see detailed discussion in Section III.A). The surface source's area should be optimized to balance geometric coverage (ensuring full specimen exposure) and computational efficiency (reducing extraneous voxels of the "surface source" that produce flux failing to intersect the specimen). Program-2 imports the "surface source" data obtained from Program-1, treating it as a tailored emission source and calculates $\phi(E)$ and $\phi_0(E)$. Example input commands for executing the sequence-calculation framework with PHITS are detailed in Appendix A.

The key advantage of our proposed framework is that Program-1, which handles the most time-consuming part of the simulation, needs to be executed only once for each experimental facility or beamline configuration. Once the surface source is generated, Program-2 can be run independently for each specific specimen, significantly reducing overall computation time when analyzing multiple specimens, as the runtime of Program-2 on a typical PC is only a few minutes per specimen. It should be noted that the statistical fidelity of Program-1's transport data is critical to ensure accuracy in Program-2, as truncation uncertainties propagate into flux and reaction rate estimates.

MC simulation results are normalized per source particle (history) with flux quantities reported relative to a single primary particle. For clarity, in electron beam-converter interaction studies, flux values are expressed in units of cm^{-2} per primary electron. Conversely, simulations utilizing the "surface source" methodology (see Program-2 in Fig. 2) report flux in units of cm^{-2} per tailored

source. In this work, approximately 10^9 particle histories were simulated to achieve statistical uncertainties below 5%.

III. Results and Discussion

A. Neutron Spectrum of "Surface Source" and Validation of the "Sequence-Calculation" Framework

In our experimental setup, 109-MeV electrons interact with the target and produce neutrons through a two-stage process. First, electrons interact with the Coulomb field of tungsten nuclei, generating bremsstrahlung radiation with a continuous energy spectrum up to the initial electron energy. Second, these photons induce photoneutron reactions, mainly (γ, n), within the conversion target material, resulting in neutron emission. Fig. 3(a) shows that most neutrons are generated at the head of the target (near the lens). As the distance from this central interaction region increases, the neutron flux gradually decreases due to geometric dispersion and attenuation effects.

Fig. 3(b) compares neutron fluxes inside the target and at the sidewall surface. The neutron flux inside the target exhibits its highest intensity in the 0.1–5 MeV energy range (red histogram in Fig. 3(b)), indicating a dominance of fast neutrons. Several dips in the spectrum between 2 eV and 2 keV mainly arise from resonance absorption in tungsten isotopes, with the most pronounced dip around 19 eV due to its elevated (n, γ) cross-section of ^{186}W. Neutrons undergo significant moderation and absorption within the target and moderator tank before reaching the sidewall, leading to considerable changes in energy distribution and intensity (blue histogram in Fig. 3(b)). At the sidewall surface, the flux shows a dominance of thermal neutrons. The sidewall neutron spectrum exhibits a Maxwellian distribution in the thermal regime (10^{-3}–0.3 eV) with a peak at 6×10^{-8} MeV, characteristic of thermal equilibrium with the water-filled moderator tank. In the epithermal regime (0.3 eV–0.1 MeV), the spectrum shows 1/E slowing-down behavior.

Fig. 3(c) depicts the longitudinal intensity variation of thermal and epithermal neutron flux along the converter' s sidewall at 10 mm intervals. The highest epithermal neutron flux is observed at distances of 40–50 mm from the front face of the converter, whereas the thermal neutron flux reaches its maximum intensity at approximately 50 mm. These calculations suggest the specimen should be installed on the sidewall at a distance of 50 mm from the front face of the converter to optimize neutron exposure. This location is hereafter referred to as the main irradiation position.

Fig. 4 shows the electron and photon fluxes at the sidewall surface, indicating that a certain amount of electrons and photons generated from interactions of 109-MeV accelerated electrons with the target reach the irradiation position (i.e., the specimen). These photons and electrons, especially those with energy higher than the neutron separation energy of specimen materials, can produce neutrons via interaction with the specimen, called secondary neutrons. As men-

tioned in Section II.B, to optimize computational resources, Program-1 records only neutrons crossing the "surface source," so $\phi(E)$ and $\phi_0(E)$ determined by Program-2 do not include secondary neutron contributions. The impact of secondary neutrons is expected to be negligible, as electron and photon fluxes at the sidewall surface are lower than those inside the target by three to four orders of magnitude, as shown in Fig. 4, and the specimen size is extremely small, as listed in Table 3.

In the following analysis, we quantitatively confirm that excluding these secondary neutrons does not significantly affect the results. We conducted additional simulations in which only electrons and photons crossing the "surface source" were recorded in Program-1 and subsequently used as the input source in Program-2. In this configuration, the neutron flux obtained in Program-2 reflects only the contribution from secondary neutrons—those produced via photon- and electron-induced reactions within the specimen itself. Fig. 5 shows that secondary neutron fluxes corresponding to the four investigated specimens are more than four orders of magnitude lower than their associated primary ones (obtained when only neutrons are recorded in Program-1). In fact, the contribution of secondary neutrons to $\phi(E)$ is less than 0.1% for all investigated specimens. Furthermore, secondary neutrons predominantly occupy energy regimes outside the thermal and epithermal ranges. This finding validates the exclusion of secondary neutron contributions, thus routine self-shielding calculations for the studied materials can be performed with a pure neutron-emitting "surface source" without sacrificing accuracy.

To fully validate the sequence-calculation approach, we compare $\phi(E)$ at the main irradiation position obtained using the "sequence-calculation" method and conventional methods in Fig. 6, showing good agreement between the two calculation approaches. Fig. 6(b) compares neutron flux ratios between the two approaches, showing an average ratio of 1.03 ± 0.19 across all energy groups.

B. Thermal and Epithermal Neutron Self-Shielding Factors

Table 5 displays G_{th} and G_{epi} for Au, Cu, W, and Zr specimens at the main irradiation position obtained using our proposed "sequence-calculation" method and the conventional approach (the latter performed using MCNP6). The G_{th} and G_{epi} values computed with PHITS and MCNP6 are in good agreement. For G_{th}, relative differences between the two codes are <3% for all isotopes, while those for G_{epi} are <6% for all isotopes. This consistency validates the robustness of both codes despite differences in their default nuclear data libraries (JENDL-4.0 vs. ENDF/B-VII.1).

To complement this conclusion and better understand the underlying spectral behavior, we further examine the energy-dependent transmission function, defined as the $\phi(E)/\phi_0(E)$ ratio, presented in Fig. 7. In the $\phi/\phi_0(E)$ spectrum of gold—a high neutron absorber (Fig. 7(a))—a pronounced dip ($\phi/\phi_0 = 0.08$) occurs in the energy groups of 4.75–5.0 eV, corresponding to strong resonance

absorption of ^{197}Au (27×10^{-3} barns at 4.9 eV). Depression in the thermal energy region reflects the dominance of absorption cross-section over scattering ($\sigma_\gamma > \sigma_s$) in this regime.

In the $\phi/\phi_0(E)$ spectrum of copper (Fig. 7(b)), minimal spectral variation is observed except near 1.9–2.1 keV, where ϕ/ϕ_0 peaks at 1.42 (1.9–2.0 keV) before declining to 0.85 (2.0–2.1 keV). As a neutron scatterer ($\sigma_s > \sigma_\gamma$), this behavior arises from resonance self-shielding, wherein neutrons near resonance energies undergo multiple scattering, delaying absorption until energy loss shifts them below resonance thresholds. A 0.1 mm zirconium foil thus introduces minimal perturbation to the neutron field, validating its use as a reference material in irradiation geometries where self-shielding corrections are unnecessary.

The transmission spectrum $\phi/\phi_0(E)$ for tungsten (Fig. 7(c)) exhibits complex energy-dependent behavior due to contributions from its isotopic composition (^{180}W, ^{182}W, ^{183}W, ^{184}W, and ^{186}W). Pronounced dips in ϕ/ϕ_0, attributed to resonance absorption, occur in the energy groups of 4.0–4.25 eV ($\phi/\phi_0 = 0.33$), 18–19 eV ($\phi/\phi_0 = 0.36$), 19–20 eV ($\phi/\phi_0 = 0.38$), 20–21 eV ($\phi/\phi_0 = 0.59$), and 21–22 eV ($\phi/\phi_0 = 0.54$). Localized increases in ϕ/ϕ_0, similar to copper' s behavior, arise from neutron scattering moderation effects prior to absorption below resonance energies. For zirconium (Fig. 7(d)), $\phi/\phi_0 \approx 1$ across all energy groups, indicating negligible self-shielding. This neutrality stems from zirconium' s low absorption and scattering cross-sections.

These results collectively support the reliability and accuracy of the computed g-factors, as evidenced by the close agreement between PHITS and MCNP6 calculations. Furthermore, detailed analysis of the energy-dependent transmission spectra demonstrates that spectral behaviors are consistent with known neutron interaction characteristics of each material, such as resonance absorption and scattering dominance. This strong alignment with physical expectations not only reinforces the credibility of the simulation results but also validates the sequence-calculation framework as a robust and efficient method for neutron field characterization, particularly for complex irradiation setups where computational optimization is critical. It is worth noting that the total computation time for all four specimens using PHITS was just about one month (including one month for Program-1 initialization and a few minutes per specimen for Program-2), compared to approximately four months with MCNP6 using conventional methods (one month per specimen). The sequence-calculation framework with PHITS enables rapid g-factor calculations for multiple specimens once Program-1 completes, requiring only a few minutes per additional specimen. Thanks to this advantage in reducing computational time, the sequence-calculation method is further employed to investigate the dependence of g-factors on specimen thickness, irradiation positions (different from the main irradiation position), and spatial variation of the neutron flux. These results are presented in Section III.C.

C. Effect of Neutron Flux Spatial Variation, Specimen Thickness, and Irradiation Position

To systematically investigate the effects of specimen thickness, irradiation position, and spatial neutron flux variation on computed g-factors, we employ Au foil as a representative material. Au is selected due to its well-known nuclear properties, including a high thermal neutron capture cross-section and prominent resonance structures, which make it highly sensitive to changes in neutron spectral characteristics. Moreover, Au is commonly used as a standard monitor material in activation experiments.

Fig. 8 presents G_{epi} and G_{th} evaluated for ^{197}Au specimens (10 mm $\times$ 10 mm foils) of various thicknesses (τ) positioned at multiple axial locations along the converter' s sidewall, represented by the axial position (D), defined as the distance from the front face of the converter to the center of the specimen. Both G_{epi} (Fig. 8(a)) and G_{th} (Fig. 8(b)) increase with decreasing τ, consistent with reduced neutron absorption in thinner specimens. However, G_{th} saturates for $\tau < 10^{-2}$ mm. G_{epi} almost plateaus between D = 20–80 mm, then declines gradually up to $D = 170$ mm (Fig. 8(a)). This trend persists for $\tau = 100$–10^{-3} mm but vanishes for $\tau = 10^{-4}$ mm, where G_{epi} remains constant across all D. G_{th} similarly plateaus at D = 20–80 mm and decreases slightly at $D > 80$ mm for $\tau = 100$ mm and $\tau = 10^{-1}$ mm (Fig. 8(b)). Notably, G_{th} exhibits plateau trends throughout investigated positions for specimens as thick as $\tau > 10^{-2}$ mm, contrasting with G_{epi} behavior for specimens as thin as $\tau < 10^{-3}$ mm.

Positional variations in G_{epi} and G_{th} (Fig. 8) arise from angular dependence in neutron incidence, driven by spatial heterogeneity of the neutron field. To quantify this effect, the angular distribution of thermal and epithermal neutrons incident on the specimen surface was resolved using a T-Cross tally with 2° angular mesh. Fig. 9(a) illustrates the azimuthal angle (θ) distribution relative to the normal vector of the specimen' s planar surface, where $\theta = 0°$ corresponds to a collimated beam perpendicular to the foil. For specimens positioned at $D = 20, 50, 80, 110, 140$, and 170 mm, polynomial fittings to the simulation data reveal dominant incidence angles of $\theta \approx 15°, 10°, 25°, 38°, 45°$ and 55°, respectively. This progression reflects geometric divergence of the neutron field. At positions around $D \approx 50$ mm, neutrons exhibit forward-biased trajectories due to proximity to the beam interaction zone, while downstream positions ($D > 80$ mm) experience broader angular spreads.

For positions $D = 20, 50$ and 80 mm, angular deviations in neutron incidence ($\Delta\theta \approx 5°$–$15°$) exert negligible impact on G_{epi} and G_{th}, resulting in minimal positional variation (Fig. 8). Beyond $D = 110$ mm (dominant $\theta \approx 38°$), neutron flux divergence becomes adequate for the effect of neutron flux spatial variation to manifest clearly. This phenomenon arises from increased effective neutron path lengths through the specimen at larger θ, enhancing absorption cross-section interactions. The observed trend aligns with prior studies, where collimated neutron beams yield higher G_{res} compared to isotropic fields.

As shown in Fig. 3(c), thermal and epithermal neutron flux intensities vary along the longitudinal axis of the converter' s sidewall due to differences in neutron migration paths from the target to specimen irradiation zones. However, simulation calculations confirm that variation in flux intensity does not alter G_{epi} and G_{th}. Fig. 9(b) illustrates energy spectra of neutron flux incident on specimens at various axial positions, resolved using a T-Cross tally with energy meshing. While absolute flux magnitudes differ across positions, spectral shapes remain nearly identical, preserving the energy-dependent neutron interactions critical to self-shielding corrections. Self-shielding factors depend primarily on the relative energy distribution of neutrons rather than absolute flux intensity.

Analysis of G_{epi} and G_{th} trends from $D = 80$ mm to $D = 170$ mm (Fig. 8) reveals distinct thickness-dependent sensitivities to neutron flux spatial variation. To quantify these effects, g-factors at $D = 170$ mm (maximal angular divergence) and $D = 80$ mm were compared as functions of specimen thickness (τ). Peak sensitivity occurs for $\tau = 10^{-2}$ mm to 3×10^{-2} mm, with relative deviations exceeding 25% (Fig. 10(a)). Deviations diminish for $\tau > 100$ mm (saturation of self-shielding) and $\tau < 10^{-4}$ mm (negligible self-shielding). A different tendency for G_{th} can be seen in Fig. 10(b). Sensitivity increases monotonically with τ, peaking at $\tau = 100$ mm (relative deviations ~13%). For $\tau < 10^{-2}$ mm, deviations fall below 2%, rendering positional effects insignificant. These divergent trends indicate that epithermal self-shielding is governed by resonance absorption in intermediate-thickness specimens, while thermal self-shielding amplifies with thickness due to cumulative path-length absorption. These results establish critical thresholds for specimen design: thinner foils ($\tau < 10^{-2}$ mm) minimize spatial sensitivity in G_{th}, while mid-range thicknesses ($\tau \approx 10^{-3}$–10^{-1} mm) require careful positioning for G_{epi} applications.

To elucidate observed trends in Fig. 10(a) and Fig. 10(b), transmission functions for specimens of critical thicknesses $\tau = 10^{-2}$ mm (epithermal-sensitive) and $\tau = 100$ mm (thermal-sensitive) were compared between $D = 80$ mm and $D = 170$ mm (Fig. 10(c) and Fig. 10(d)). For $\tau = 10^{-2}$ mm, spatial flux variation predominantly impacts the resonance energy region, where ϕ/ϕ_0(4.75–5.0 eV) differences between positions exceed 30% (Fig. 10(c)). For $\tau = 100$ mm, ϕ/ϕ_0(< 0.5 eV) differences concentrate in the thermal region, with deviations >17% (Fig. 10(d)), explaining the pronounced positional dependence of G_{th} for thick specimens. These results validate thickness-dependent spatial sensitivities, emphasizing the need for geometry-specific corrections in high-precision activation analysis.

Neutron self-shielding corrections depend on both intrinsic material properties (composition, density, thickness) and extrinsic factors such as spatial characteristics of the neutron field. In this section, critical specimen thicknesses for thermal/epithermal neutron self-shielding spatial sensitivity were identified. Thinner foils minimize spatial sensitivity in the thermal region while mid-range specimen thicknesses ($\tau \approx 10^{-3}$–10^{-1} mm) maximize spatial sensitivity in the epithermal region. These findings underscore the necessity of position- and

thickness-dependent corrections in high-precision NAA, particularly for facilities with non-uniform neutron fields.

IV. Conclusion

This work presents a significant advancement in computational methodology for neutron self-shielding analysis in indirect neutron generation facilities, such as those generated by high-energy accelerated electron beams. By introducing a two-stage "sequence-calculation" framework, the study overcomes the high computational cost of conventional Monte Carlo simulations for multiple specimens. The separation of the simulation into Program-1 and Program-2 effectively decouples the time-intensive neutron source generation, which originates from interactions of high-energy electrons with target nuclei, from specimen-specific flux calculations, allowing the latter to be performed rapidly and efficiently without sacrificing accuracy.

The framework' s ability to preserve detailed spatial and spectral fidelity, along with its demonstrated accuracy through cross-code validation using PHITS and MCNP6, confirms its suitability for routine applications in complex irradiation environments. The proposed method has been applied to calculate thermal and epithermal neutron self-shielding factors for Au, Cu, W, and Zr specimens for an electron-beam-driven neutron source—the IREN facility at the Joint Institute for Nuclear Research (JINR) in Dubna, Russia. These values will be employed in upcoming research at this facility.

We also investigated the effects of specimen thickness and spatial neutron flux variation on self-shielding factors, identifying key sensitivities and highlighting the necessity of geometry-specific corrections. This task requires extensive computational resources and would be impractical without the proposed sequence-calculation framework. Eventually, the proposed sequence-calculation framework is not limited to neutron self-shielding factors but can be applied to a wide range of radiation transport problems involving complex geometries and source terms, offering a versatile and efficient tool for advanced simulations.

V. Acknowledgments

The authors acknowledge partial support from the Vietnam Ministry of Science and Technology for financial support through Grant DTCB.06/25/TTDTHN. The support from the Plenipotentiary of Vietnam to JINR for our collaboration is highly appreciated.

VI. Declaration of Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

VII. Declaration of Generative AI in Scientific Writing

No AI or AI-assisted technology was used to prepare this academic manuscript.

VIII. Author Contributions

Viet-Huy Le: Writing - Original Draft, Writing - Review & Editing, Conceptualization, Methodology, Investigation, Formal analysis, Validation, Visualization, Data Curation
Tien-Thanh Pham: Investigation, Formal analysis, Data Curation
Hong-Khiem Le: Writing - Review & Editing, Supervision, Conceptualization, Resources
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References

[1] A. Trkov et al., On the self-shielding factors in neutron activation analysis. Nucl. Instrum. Methods Phys. Res., Sect. A 610, 553-565 (2009). doi: 10.1016/j.nima.2009.08.079
[2] J. Salgado, I. Goncalves, E. Martinho, Epithermal neutron self-shielding factors in foils for collimated beams. Appl. Radiat. Isot. 60, 677-681 (2004). doi: 10.1016/j.apradiso.2003.10.012
[3] I. Goncalves, E. Martinho, J. Salgado, Monte Carlo calculation of epithermal neutron resonance self-shielding factors in foils of different materials. Appl. Radiat. Isot. 56, 945-951 (2002). doi: 10.1016/S0969-8043(02)00055-6
[4] I. Goncalves, E. Martinho, J. Salgado, Monte Carlo calculation of epithermal neutron resonance self-shielding factors in wires of different materials. Appl. Radiat. Isot. 55, 447-451 (2001)*. doi: 10.1016/S0969-8043(01)00089-6
[5] I. Goncalves, E. Martinho, J. Salgado, Monte Carlo calculation of resonance self-shielding factors for epithermal neutron spectra. Radiat. Phys. Chem. 61, 461-462 (2001)**. doi: 10.1016/S0969-806X(01)00300-0
[6] I. Goncalves, E. Martinho, J. Salgado, Extension to cylindrical samples of the universal curve of resonance neutron self-shielding factors. Nucl. Instrum. Methods Phys. Res., Sect. B 213, 186-188 (2004). doi: 10.1016/S0168-583X(03)01550-7
[7] E. Martinho, I. Goncalves, J. Salgado, Universal curve of epithermal neutron resonance self-shielding factors in foils, wires and spheres. Appl. Radiat. Isot. 58, 371-375 (2003). doi: 10.1016/S0969-8043(02)00313-5

[8] E. Martinho, J. Salgado, I. Goncalves, Universal curve of the thermal neutron self-shielding factor in foils, wires, spheres and cylinders. J. Radioanal. Nucl. Chem. 261, 637-643 (2004). doi: 10.1023/B:JRNC.0000037107.17274.16
[9] J. Boettcher et al., The LUE-200 accelerator at the IREN facility: Current status and development. Phys. Part. Nucl. Lett. 11, 665-671 (2014). doi: 10.1134/S1547477114050069
[10] K. Shibata et al., JENDL-4.0: A New Library for Nuclear Science and Engineering. J. Nucl. Sci. Technol. 48, 1-30 (2011). doi: 10.1080/18811248.2011.9711675
[11] J. Kulesza et al., MCNP Code Version 6.3.0 Theory & User Manual. Los Alamos National Laboratory Tech. Rep. LA-UR-22-30006 (Rev. 1. Los Alamos, NM, USA, 2022). doi: 10.2172/1889957
[12] T. Sato et al., Features of Particle and Heavy Ion Transport Code System (PHITS) version 3.02. J. Nucl. Sci. Technol. 55, 684-690 (2018). doi: 10.1080/00223131.2017.1419890
[13] P. Treado, P. Chagnon, Neutron-capture gamma-ray spectra of the tungsten isotopes. Nucl. Phys. 34, 623-627 (1962). doi: 10.1016/0029-5582(62)90011-1
[14] T. Soto-Bernal et al., Neutron production during the interaction of monoenergetic electrons with a Tungsten foil in the radiotherapeutic energy range. Nucl. Instrum. Methods Phys. Res., Sect. A 868, 27-38 (2017). doi: 10.1016/j.nima.2017.06.027

Appendix A: Examples of Input Commands for Important Parts in "Sequence-Calculation" Framework (Execution Using PHITS Code)

Table A. Optioning "surface source" for recording particle transport data (for Input 1 of Program-1 in Fig. 2).

Input command	Description
[T-Cross]	Tally type for recording particle transport data through "surface source"
mesh = reg	Mesh type is region-wise
reg = 1	Number of crossing regions
non = Intersection of cell A (converter' s case) and cell B (a void cell interfaces with the converter' s sidewall) results in a "surface source" with an area S.	
r-from =	
r-to =	
area =	
e-type = 1	Custom energy mesh
ne = 640	Number of energy mesh points

Input command	Description
infl: {640_{{{group}}*{{energy}}}*{structure}.txt} [1-640]	Sub-file contains 640-group energy structure (MATSSF database)
unit = 1	Unit is [1/cm^2/history]
output = flux	Surface crossing flux
dump = -11	Number of physical quantities to be recorded, <0: ascii, >0: binary
file = cross_{{{particle}}*{{transport}}*{data}.out	Output file restoring particle transport data

Table B. Assessing statistical accuracy of the "surface source" (for Input 1 of Program-1 in Fig. 2).

Input command	Description
[T-Cross]	Tally type for assessing statistical accuracy of particle transport data of "surface source"
mesh = reg	
reg = 1	
non =	
r-from =	
r-to =	
area =	
e-type = 1	
ne = 640	
infl: {640_{{{group}}*{{energy}}}*{structure}.txt} [1-640]	
unit = 1	Unit is [1/cm^2/history]
output = flux	Surface crossing flux
axis = eng	Axis of output is energy distribution
part = neutron electron photon	Type of particle desired for statistical accuracy assessment
file = check_{statistical}.out	Output file for assessing statistical accuracy of particle transport data

Table C. Defining emission source using the "surface source" as a tailored emission source (for Input 2 of Program 2 in Fig. 2).

Input command	Description
[Source]	Section for definition of emission source
s-type = 17	Source type for reusing "surface source" as a tailored emission source
file = cross_{{{particle}}*{{transport}}}*{data}.out dump = -11	Particle transport data restored from Output 1 of Program-1
part = neutron (or photon/electron)	Selection of type of particle emitting from tailored emission source
idmpmode = 0 (or = 1)	= 0: Each particle data recorded in the "surface source" file is treated as an independent history. = 1: Particle data in the "surface source" file are processed by taking account of particle correlations in the previous step.

Note: Figure translations are in progress. See original paper for figures.