Mathematical formulae for neutron self-shielding properties of media in an isotropic neutron field

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Abstract

In the current study, an \textit{ab initio} derivation of the neutron self-shielding factor to solve the complex neutron transport problem of the decrease of the neutron flux as it penetrates into a material placed in an isotropic neutron field having equal flux in all directions. The theory of steady-state neutron transport was employed, starting from Stuart’s formula, to derive simple analytical formulae based on the integral cross-section parameters. The formulae could be adopted by the user according to various variables, such as the neutron flux distribution and geometry of the simulation at hand. The concluded formulae of the self-shielding factors comprise an inverted sigmoid function normalized with a weight representing the ratio between the macroscopic total and scattering cross-sections of the medium. The general convex volume geometries are reduced to a set of chord lengths, while the neutron interaction probabilities within the volume are parameterized to the epithermal and thermal neutron energies. The arguments of the inverted-sigmoid function were derived from a simplification of neutron transport formulation. The derived analytic formulae agreed greatly with the experimental observations for different elements and geometries.

1. Introduction

Over time, neutron activation analysis has been evolving into a very effective nuclear analytical technique. Such techniques are often utilized for non-destructive elemental concentration measurement in unknown materials (instrumental neutron activation analysis) and nuclear material interrogation [1, 2]. The constraints include neutron fluence, the fraction of fluence that reaches the interior of the sample, sample mass, and sample geometry [3–12]. Furthermore, the neutron’s energy spectrum is varied, but ideally suited to research using the ideal Maxwellian distribution at room temperature, while the other distributions must be altered to match the reference nuclear reaction data [3, 7, 13]. Apart from that, neutrons are deeply employed in two significant geometries, including but not limited to: (1) beam geometry, where the neutron currents are assumed to travel in one direction, and (2) field geometry, where neutrons impact the sample from all directions, presuming the field is isotropic and has equal flux densities from all directions [14–16]. There is an important functional difference between these two geometries, i.e., the effect on the neutron flux itself. For instance, when exposing a sample to a neutron beam, the interior of the sample will be exposed to an altered radiation field, a lesser neutron fluence than the exterior part, in all circumstances, regardless of the geometry of the neutron source. This phenomenon is known as self-shielding, and it is a critical element of the neutron transport phenomenon. In the case of field geometry, the net neutron current essentially disappears, while the fluence (or flux) becomes the observable quantity. There is an interplay between neutron absorption in the sample and the overall neutron flux [15].
Predominantly, the correlation between neutron self-shield factors and the set of parameters involved in the calculation of its value had been studied by several scientists [17–27], who gave dimensionless variables to identify and encompass the physical and geometric varieties of the sample geometries in order to attain a universal formula for self-shielding. The Monté-Carlo approach effectively calculates self-shielding, but it takes time and an experienced user to achieve acceptable accuracy and efficiency [28], see A. Empirical expressions, such as those given by researchers in [19–23] based on [17] have been derived for a few specific geometries and a limited number of elements.

Herein, we present a complete investigation of the neutron self-shielding phenomenon in different media. Additionally, a full description of the physics behind the theme was provided, taking into consideration the neutron transport inside the sample and the absorption and scattering phenomena as a function of neutron energy. In that objective, the problem was transformed from a spectroscopic set of parameters, usually unreachable for the common user, to an integrated set of well-known parameters and factors. The use of detailed spectroscopic parameters, such as ENDF data, cross-section, detailed dimensions and shapes, the widths of neutron resonances for either scattering or absorption, etc, requires time and experienced users to make use of them with acceptable accuracy and efficiency, the cost most scientists cannot afford to just calculate a single parameter in their routine work. Our intention is focused on avoiding such cost and enhancing present formulae and using an integral set of well-known parameters such as thermal cross-section, resonance integral, and average chord length. All remaining factors are calculated from these three parameters. Though the existence of a mathematical formulation of self-shielding in materials of different geometries and compositions shall deliver additional tools to improve the precision of reaction parameters and activation analysis calculations.

### 2. Materials and methods

Experimentally measured and theoretically calculated data were collected from different sources for the self-shielding factor in In, Au, Co, Cu, and Fe samples. The geometries for these elements were foils, wires, and additional tools to improve the precision of reaction parameters and activation analysis calculations.

#### 2.1. Uncertainty

The uncertainty of digitized experimental data was difficult to determine due to the use of different linear and logarithmic scales in old graphs and the dependence among them. Determining the exact value is impossible due to the extent of the symbol in the area of the graph. There was additional uncertainty in the digitized data resulting from the size of these symbols relative to the range of the reported results in these works. We used the following formula: 

$$\sigma = \sigma_X + \sigma_Y,$$

where \(\sigma_x\) and \(\sigma_y\) are the dependent uncertainties in the digitized \(X\) and \(Y\) coordinates in the original graph accompanying these older publications. The typical value of digitization in the uncertainty of experimental data was less than 2%, which was added to the reported uncertainty as a dependent

| Isotope | \(\sigma_t\) | \(\sigma_s\) | \(\sigma_a\) | \(\sigma_r\) | \(I_t\) | \(I_s\) | \(I_a\) | \(I_r\) |
|---------|------------|------------|------------|------------|--------|--------|--------|--------|
| Na      | 0.528      | 3.3929     | 0.528      | 3.9209     | 0.3021 | 130.81 | 0.3021 | 131.11 |
| Mn      | 13.275     | 2.1163     | 13.275     | 15.391     | 13.168 | 621.33 | 13.168 | 634.5  |
| Fe      | 2.5615     | 11.35      | 2.5615     | 13.912     | 1.2706 | 127.09 | 1.2706 | 128.36 |
| Co      | 37.173     | 6.0319     | 37.173     | 43.204     | 74.78  | 791.53 | 74.78  | 866.31 |
| Cu      | 3.7531     | 7.8424     | 3.7531     | 11.595     | 4.0309 | 129.89 | 4.0309 | 133.93 |
| In      | 194.07     | 2.5686     | 194.07     | 196.64     | 3088.5 | 214.12 | 3088.5 | 3302.6 |
| Au      | 98.672     | 7.9298     | 98.672     | 106.6      | 1567.9 | 405.52 | 1567.9 | 1973.4 |

### Table 1. Element-averaged cross-section and resonance integral data. \(\sigma_t, \sigma_s, \sigma_a, \sigma_r\) are the capture, scattering, absorption and total cross-sections at thermal energies. Similarly, \(I_t, I_s, I_a, I_r\) are the capture, scattering, absorption and total resonance integral at epithermal energies. Data are obtained from the integration of the cross section over an ideal Maxwellian neutron field and epithermal neutrons having shape parameter \(\alpha = 0 [9, 10]\).
variable, if available. There is another source in the experimental measurements uncertainty made on infinite wire or foils, which was not mentioned in the literature, the systematic bias towards a higher value of the neutron self-shielding factor as a result of the experimental infeasibility of conducting the experiments on infinite samples. This bias shall be clarified in the discussion.

3. Results and discussion

According to Stuart [45], the old quantity for an absorbing body is its neutron blackness,

$$\beta = \frac{j_{\text{in}} - j_{\text{out}}}{j_{\text{in}}}$$

(1)

based on the neutron current density entering the body \((j_{\text{in}})\) or going out of it \((j_{\text{out}})\). Stuart [45] had derived the formula for \(\beta\) based on variational principle and assuming a uniform isotropic neutron field with scattering that does not change the energy spectrum on the neutrons (change of energy is treated as absorption). Blaauw [18, 46, 47] began with Stuart’s formula [45];

$$\beta = \frac{\sum_{\ell=0}^{\infty} \rho_{\ell}}{1 - \sum_{\ell=0}^{\infty} \left(1 - \frac{1}{2\ell+1}\right) \rho_{\ell}}$$

(2)

Here, \(P_0\) is the probability of the first interaction derived from the transport kernel [45, 46] in steady-state.

$$P_0 = \frac{\sigma_t}{S} \int_V \Pi_0(r) d\bar{r},$$

(3)

where \(\Pi_0(\bar{r})\) is the unscattered flux within the material;

$$\Pi_0(\bar{r}) = 4 \int_S (\bar{n} \cdot \bar{X}) g(\bar{r}, \bar{r}') dS,$$

(4)

Here, \(\bar{n}\) and \(\bar{X}\) are unit vectors in the direction of the normal to the surface and the neutron wavevector, respectively. The point symmetry neutron collision kernel has the form of Green’s function [27, 48–50]:

$$g(\bar{r}, \bar{r}') = \frac{\exp(-\sum_{\ell} |\bar{r} - \bar{r}'|)}{4\pi |\bar{r} - \bar{r}'|^2},$$

(5)

that gives the probability a neutron shifts between phase-space coordinates \(\bar{r}\) and \(\bar{r}'\) in one collision point geometry. Time reversal is applied in such cases by interchange, or \(\bar{r}\) and \(\bar{r}'\), i.e., moving in reverse direction. In general, other geometries had asymptotic form as point-like geometry [27, 49]. The value of \(\Pi_0(\bar{r})\) equals 4 in case of the nonexistence of the material in the medium because in equation (4) becomes unity. The time reversal condition is the constraint that must be satisfied by the transport kernels in all geometries. Multiple collision probability may be obtained through recursive relation [45]

$$P_n = 1 - \frac{\int_V \Pi_{n-1}(\vec{r}) \Pi_n(\vec{r}) d\vec{r}}{4 \int_V \Pi_{n-1}(\vec{r}) d\vec{r}},$$

(6)

$$\Pi_n = \frac{1}{\bar{\ell}} \int_S \Pi_{n-1}(\vec{r}) g(\vec{r}, \vec{r}') dS,$$

(7)

The value of \(\bar{\ell}\) is the average of Chord Length Distribution (CLD) may be weighed with the cosine of the angle between the chord and the normal to the surface,

$$\bar{\ell} = \frac{\int_0^{\pi/2} \int_0^{\pi/2} V(\vec{r}, \vec{\theta}, \phi) \cos(\vec{\phi}) d\vec{d}\phi}{\int_0^{\pi/2} \int_0^{\pi/2} S(\vec{r}, \vec{\theta}, \phi) \cos(\vec{\phi}) d\vec{d}\phi},$$

(8)

Here, \(S_{i,j}\) is the surface area perpendicular to the direction of the neutron. The value of the mean CLD for a convex body is related to the first Cauchy formula [51] of the integration for cylindrical shapes, which comprises \(4\sqrt{V}/S\) [32, 53], where \(S\) is the surface area enclosing a volume \(V\). This value may be used as the upper limit of one of the integrations. Note that the coordinate variables were underlined in order to avoid confusion among symbols.

There was an equivalent definition of the sample blackness [18], the self-shielding factor was denoted \(G_{\text{energy domain}}\), which is defined as the ratio between the volume-averaged fluence rate within the material’s volume that may absorb or scatter neutrons and the fluence rate within the same volume considering the absence of the interaction with neutrons. According to Blaauw [18],
The higher order terms were introduced by Blaauw [18] for extended neutron velocity distributions—denoted here $\mathcal{R}$. Remembering that the $G_{\text{(energy domain)}}$ is a neutron energy-specific parameter, any perturbation of the neutron energy distribution shall affect the experimental results as discussed in earlier work [15].

### 3.1. Mathematical model

In accordance with the previous constraint of self-shielding formulae, we shall use equation (2), include the high order in equation (9), and use the relation of blackness and self-shielding [46] (i.e. $\Sigma_t \cdot \tilde{E} = \beta$ as a first approximation). The combined formulae comprises:

$$G_{\text{(energy domain)}}(\ell) = \frac{1}{1 + \Sigma_t \cdot \frac{\tilde{E}}{P_0} \left( \frac{\Sigma_0}{\Sigma_t} \right)} + \mathcal{R}.$$  

(10)

The value of $\mathcal{R}$ was found to have negligible contributions except when relying on the entire range of Maxwellian thermal neutron distribution, as proven in appendix B. However, and for the practical of constraining the thermal neutron energy range by the cadmium cutoff energy around 0.5 eV, this term can be neglected. Hence,

$$G_{\text{(energy domain)}}(\ell) = \frac{1}{1 + \Sigma_t \cdot \frac{\tilde{E}}{P_0} \left( \frac{\Sigma_0}{\Sigma_t} \right)}.$$  

(11)

The value of $G_{\text{(energy domain)}}$ in equation (11) must be less than 1, i.e. under the condition:

$$\Sigma_t \leq \Sigma_t + \frac{\Sigma_t \cdot \tilde{E}}{P_0} \Sigma_0$$  

(12)

i.e. the parameters in the first term in equation (11) must satisfy the condition.

$$\frac{\Sigma_t \cdot \tilde{E}}{P_0} \geq 1.$$  

(13)

Precise choice of the value of $P_0$ is given in section 3.3.

Equation (11) can be rewritten as follows:

$$G_{\text{(energy domain)}}(\ell) = \left( \frac{\Sigma_0}{\Sigma_t} \right) \times \frac{1}{1 + Z}.$$  

(14)

where

$$Z = \frac{\chi(\Sigma_t)}{\Omega(\tilde{E}, \Sigma_0, \Sigma_t, \Sigma_1, \Sigma_2, \eta(\Sigma_{a1}, \Sigma_{a2}))}.$$  

(15)

The factor $\left( \frac{\Sigma_0}{\Sigma_t} \right)$ represents the total macroscopic cross-section to the macroscopic scattering cross section, i.e. it increases as the neutron absorption increases and always greater than 1. The dimensionless parameter, $Z$, is expressed as a product of three functions, macroscopic cross-section function ($\chi = \Sigma_0$) in the units of $[\text{cm}^{-1}]$ which depends on the isotopic content of the sample, geometry function ($\Omega = \frac{\tilde{E}}{P_0}$) as a function of the dimensions of the sample in the unit of $[\text{cm}]$, and a dimensionless neutron energy correcting factor ($\eta = \frac{\Sigma_{a1}}{\Sigma_{a2}}$) which is a function of the neutron absorption and the scattering cross-sections. The neutron-chord length is not the only parameter in the transport equation that depends on geometry; the first and higher-order interaction probabilities, i.e., $P_0$, are also dependent on both geometry and medium contents. These are the fundamental morphological descriptors of the medium that describe the mean intercept length and relative to the mean free-paths of neutrons within the medium. Here, $\Omega$ contains the factor of a shift in the Euclidean distance value and reflecting the total distance of interest within the medium, while $\chi$ and $\eta$ determine the slope of the steeping part of the curve.

Macroscopic cross-section function is expressed as

$$\chi(E_0) = \Sigma(E_0, E_2) = \frac{\rho N_0 \theta \sigma}{M}.$$  

(16)
where $N_A$ is the Avogadro’s number [mol$^{-1}$], $\rho$ is the density of the material [g cm$^{-3}$], and $M$ is its atomic mass [g mol$^{-1}$]. $\theta_i$ is the isotopic abundance of the absorbing isotope in which it should be multiplied by the fraction of the element in the material if a compound material is used. Here, $\bar{\sigma}$ is the integral cross-section in the energy domain between $E_1$ and $E_2$. For practical purposes, the thermal neutron energy range is bounded by the cadmium cutoff energy around 0.5 eV while the epithermal range extends from 0.5 to a few MeVs [3, 7, 10]. Here, $\sigma_i(E_n)$ is the $i^{th}$-isotope’s cross-section for the reaction channel $\iota$ at the neutron energy $E_n$ in this energy domain [cm$^2$]. In the case of compounds, this formula becomes a summation over $i^{th}$-isotope.

The $\eta$ term is the absorption to scattering ratio;

$$\eta(\Sigma_s, \Sigma_a) = \frac{\Sigma_s}{\Sigma_a}$$

In general, values of thermal cross-section and resonance integral are well known from tables [10, 54, 55] or integration of spectroscopic cross-section [9].

### 3.2. The geometry factor

The geometry factor depends on the neutron-chord length and the probability of interaction as;

$$\Omega(\text{shape parameters}) = \frac{\bar{\rho}}{P_0}$$

There were great efforts to parameterize this factor over the years. Recent efforts have been made by Trkov et al [53], especially in the extended range of neutron resonances.

In integral geometry, obtaining the orientation-dependent chord lengths of a convex body, in general, is a complicated mathematical argument; most researchers treat the problem with the body that has the minimal volume in a class of convex bodies having the same dimensions [56]. As long as we want to escape the rigorous derivations of the average neutron-chord length (cf [52, 57–61] for details), we shall use a simple formulation of the average neutron-chord length based on the fact that the trajectories of the incident isotopic neutrons traverse different lengths within the body due to scattering. The derivation proceeded under this assumption, in which the convex bodies are in an isotropic neutron field, which is the geometry that most materials have.

Considering an Euclidean space ($\mathbb{E}^3$) where the irradiated body is located with a center-of-mass at the origin of the coordinate system. The three coordinate vectors are in orthogonal directions—denoted 1, 2, and 3. The orientations of these coordinates were chosen as follows: At least one of these vectors (1) shall intersect the body surface in the direction of the shortest length between the center-of-mass (at the $\mathbb{E}^3$ origin) and a point on the surface of the body, see figure 1. The next coordinate vector (2) shall lay in a plane perpendicular to the first one to the shortest point on the body surface. The third coordinate vector (3) shall be perpendicular to the plane containing the first and second vectors and have a length equal to the distance to the surface. The lengths of the distances between the center-of-mass and the actual surfaces along the coordinate vectors are denoted $L_1$, $L_2$, and $L_3$, in their respective order. Due to scattering, the coordinates are transformed into another virtual coordinate system that is suitable to the situation and the shape on hand. The distances traveled by the neutron along the new virtual coordinate system in the body are the neutron-chord lengths, denoted $\ell_1$, $\ell_2$, and $\ell_3$, which need to be determined using transport equations. The average neutron-chord length is taken, in the present work, as the harmonic mean of these three distances; i.e.
Here, \( \bar{\ell} \) is the average neutron-chord length.

Due to symmetry operations in the diffusion equation, we shall take the condition that if there were a boundary in the difference-problem of equations 21, 22 and 24 is considered a vacuum boundary [62]. Under this condition, the boundary in the difference-problem of equations 23 and 24 is considered a vacuum boundary [62]. At the specific boundary vector \( \mathbf{r}_b \), the flux becomes \( \phi(\mathbf{r}_b) = \phi_0 \), or, according to equation 22,

\[
\phi(\mathbf{r}_b) = 0
\]  

(28)

The solution of equation (25), as derived in appendix C.1 for cartesian coordinates, resembles:

\[
\phi(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \text{Const.} e^{-i\mathbf{k}_1 \cdot \mathbf{x}} e^{-i\mathbf{k}_2 \cdot \mathbf{y}} e^{-i\mathbf{k}_3 \cdot \mathbf{z}}
\]  

(29)

Note that the coordinate variables are underlined from now on in order to avoid confusion among symbols. In order to satisfy the condition equation (28), the values of \( \ell_i \) should be related to the measurable coordinate dimensions as follows: \( \ell_1 = 2L_1 \), \( \ell_2 = 2L_2 \) and \( \ell_3 = 2L_3 \). As presented in figure 1, \( L_1 = W/2 \), similarly all other dimensions. i.e.

\[
\ell = \ell_1 \left( \frac{1}{W} + \frac{1}{D} + \frac{1}{H} \right)^{-1}
\]  

(30)

Note that for infinite foils and sheets, there is only one measurable length exits, the thickness with \( L_1 = t/2 \), \( L_2 = \infty \), and \( L_3 = \infty \) making \( \ell_1 = t, \ell_2 = \infty, \ell_3 = \infty \), and

\[
\frac{1}{\ell} = \frac{1}{3} \left( \frac{1}{\ell_1} + \frac{1}{\ell_2} + \frac{1}{\ell_3} \right)
\]  

(20)
The condition in equation (25) becomes:

\[ \phi(\mu, \phi, \rho) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_{mn} J_m(\sqrt{n^2 + B_1^2 \rho}) \times \cos m\phi e^{-\sqrt{n^2 - B_1^2 z}}, \quad \text{if} \quad n^2 > B_1^2, \]

\[ = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_{mn} J_m(\sqrt{n^2 + B_2^2 \rho}) \times \cos m\phi \cos \sqrt{B_2^2 - n^2 z}, \quad \text{if} \quad n^2 \leq B_2^2 \]

where \( J_m \) is Bessel functions of the first kind, \( C_{mn} \) is a constant and \( m \) and \( n \) are integers. Generally, \( m = 0 \) and \( n = 0 \) have the largest contribution. Hence

\[ \phi(\mu, \phi, \rho) \approx C_{00} J_0(B_1 \rho) \cos B_2 \phi \]

The first root of \( J_0 \) in equation (33) is when the argument \( B_1 \rho = 2.4048 \) while the root of the cosine function is when its argument \( B_2 \phi = \frac{\pi}{2} \). In order to satisfy the condition equation (28):

\[ \ell_1 = \frac{\pi}{2.4048} L_1 = \frac{\pi}{2.4048} R \]

\[ \ell_2 = 2L_2 = H, \]

sand none-existence of \( \rho \) dependence equation (33) gives \( \ell_3 = \infty \). i.e.

\[ \bar{\rho} = \frac{3\pi RH}{2.4048H + \pi R} \]

Note that for a finite disk of the radius \( R \) and the thickness \( t \).

\[ \bar{\rho} = \frac{3\pi Rt}{2.4048t + \pi R} \]

For infinite wire and cylinders, there is only one measurable coordinate length, the radius \( R \)

\[ \bar{\rho} = \frac{3\pi R}{2.4048} = 3.9191 R \]

The solution of equation (25), as derived in appendix C.3, for spherical shape resembles;

\[ \phi(\zeta, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} C_{lm} j_l(B_1 \zeta) P_l^m(\cos \theta) \cos m\phi, \]

where, \( P_l^m(\cos \theta) \) is the associated Legendre polynomial, \( j_l(B_1 \zeta) \) is the spherical Bessel function, and \( C_{lm} \) is the integration constant. Again \( C_{00} \) has the largest contribution. Hence

\[ \phi(\zeta, \theta, \phi) \approx C_{00} j_0(B_1 \zeta) P_0^0(\cos \theta) \]

The condition in equation (28) is satisfied if the argument of the spherical Bessel function \( (B_1 \zeta) \) equals the root of the spherical Bessel function at \( \zeta \); i.e. the condition is satisfied if \( \ell_1 = L_1 = R \). Here, \( P_0^0(\cos \theta) = 1 \) and due to symmetry of the body, there exists none-\( \zeta \) dependence which reveal \( \ell_2 = \infty \), while none-\( \phi \) dependence requires \( \ell_3 = \infty \); i.e.

\[ \bar{\rho} = 3R \]

For any other irregular shape, the average neutron-chord length can be calculated in the same manner using box geometry as approximation. Table 2 shows a comparison between our simple procedure and others.

The average neutron-chord length is larger than the dimensions of the body due to the irregular path of neutrons in the body’s material. For a sphere with a radius \( R \) is \( \bar{\rho} = 3R \), not the value of \( 2R \), while for infinite foil it is also three times its thickness, not the value of 1.5t, due to the average of the cosine in the neutron scattering path length inside the volume. However, when Sjostrand et al [63] calculated the average neutron-chord length for a sphere assuming an isotropic flux distribution, the result was equal to the radius \( R \) due to the use of different weighting factors.

### 3.3. Probability of the neutron interaction

The next step is to obtain a mathematical formula for the probability of a single interaction within the volume \( (P_0) \), i.e., the probability that a neutron will suffer at least one more interaction. In the case of thermal energies, the domain of the Maxwellian distribution below the cadmium cut-off energy may be considered as that of the averaged energy at 0.025 eV for which scattering and multiple scattering shall not disturb the overall neutron energy distribution [64]. The neutron absorptions are the result of the various neutron resonances that are
Table 2. The geometry factor $\Omega(\vec{\ell}, \Sigma)$ deduced from simple convex geometries presented in figure 1 in comparison to reported factors from different researches. Reported factors are from [19, 20, 22, 23].

| Shape      | Dimensions | The geometry factor $\Omega(\vec{\ell}, \Sigma)$ |
|------------|------------|-----------------------------------------------|
| Sheet-     | $t$        | $3t/P_0$                                      |
| infinite   |            | $1.5t$                                        |
| Disc       | $t, R$     | $3t/R$                                        |
|            |            | $-\infty$                                     |
| Box/Slap   | $H, W, D$  | $3R/\exp(\frac{3H}{R} + \frac{3D}{R})$      |
| Sphere     | $R$        | $1.65R/\exp\left(\frac{R}{H} + \frac{R}{W}\right)$ |
| Cylinder   | $R$        | $3.9191R/P_0$                                 |
| Cylindrical|            | $-\infty$                                     |
| General shape | $L_1, L_2, L_3$ | $\frac{3}{P_0} \left(\frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3}\right)^{-1}$ |
|            |            |                                              |

predominant in the epi-thermal region, including those of capture and possible fission components while scattering components cause the escape of neutrons from this region.

The neutron-escape probability, the factor $p$ in reactor physics, measures the fraction of neutrons that have escaped absorption and still exist after having been slowed down from their epi-thermal energies to—say thermal energies—due to these ‘resonance traps’ and reduces the absorption losses [65, 66]. Several authors have tried to calculate the resonance escape probabilities from the first principles [66–69] while others calculate them directly from the thermal utilization factor of reactors (cf. [70]).

In the present work and under the condition in equation (13), the probability of interaction is obtained from the attenuation relation ($\phi = \exp(-\Sigma_\alpha \times \text{mean distance})$). The scattered neutron continues to exist within the body. The mean travelled distance is the averaged neutron-chord length, which allows us to write directly and according to Rothenstein [66], and for approximation, the following

$$P_0 \sim (1 - \exp(-\Sigma_\ell \vec{\ell})),$$

which satisfies the condition in equation (13). In the extended range of epi-thermal neutrons, the flux varies as $1/E_n$ from cadmium cut-off energy at 0.5 eV to the end of the neutron spectrum—say 1 MeV. Multiple scattering disturbs the energy distribution by reducing the number of neutrons in the epi-thermal region. In reactor physics, this phenomenon is described by the resonance escape probability, which is the probability that a neutron will slow down from fission energy to thermal energies without being captured by a nuclear resonance. This phenomenon depends on the diffusion properties of the medium. In the comparison given in figure 3, the values of $G_{epi}$ vary as in equation (42) but $\vec{\ell}^{2/3}$ replaces $\vec{\ell}$. There was no clear reason for this dependence.

However, there is a simple experimental remark in neutron physics: whenever the neutron energy distribution repudiates the proper thermalization distribution (Maxwellian + $1/E$ dependence in the epi-thermal region) by any mean such as absorption, the neutrons rapidly redistribute their velocity population within the diffusion distance to follow the proper distribution—up to thermalization. [2, 71, 72]. To compensate for such dependence, in the present work we introduced a parameterized factor to enhance the formula in equation (42) in the epi-thermal range as follows:

$$P_0 \sim \frac{1}{P_{\text{escape}}} (1 - \exp(-\Sigma_\ell \vec{\ell} P_{\text{escape}})),$$

where

$$P_{\text{escape}} = 2 \sqrt{\frac{\Sigma_\alpha - \Sigma_\ell}{\Sigma_\alpha}} \frac{\vec{\ell}}{\sqrt{\Sigma_\ell \vec{\ell}}}$$

which, also, satisfies the condition in equation (13).

The subscript (energy domain) is to be replaced by ‘th’ in case of thermal neutron energies below cadmium cutoff energy (~0.5 eV) or by ‘epi’ for epi-thermal neutrons having energy domain greater than the cadmium cutoff energy. Here, we have used two notions of flux $\varphi_{\text{th}}$ and $\varphi$ which stand for unperturbed neutron flux for which the material is diluted or absent [73] and the measured self-shielded neutron flux in the vicinity of the material, respectively.
3.4. Verification with experiment

The obtained mathematical values with the present ab initio model were compared with the experimental values in figure 2. The exact parameters of the experimental data, such as foil thickness, wire radius, and cylinder height were obtained from the original sources (whether these were literature or our previous experiments). In the thermal energy range, the derived formula in equations (14) and 42 gave a good representation of the experimental data for In, Au, and Co within the experimental uncertainty, whether it was wires or foils.

In the epi-thermal region, the integral cross-section of equation (17) is replaced by the resonance integral. Table 1 contains the element-averaged resonance integrals for the 1/E averaged neutron distribution together with the thermal cross-section data based on the Maxwellian distribution of neutron energies for capture reactions [10] and scattering reactions [9]. These integral data were used to calculate the epi-thermal self-shielding factor, $G_{\text{epi}}$, and are represented by lines in figure 3. Experimental results from the literature of Figure 2.

Comparison of $G_{\text{th}}$ of our approach with Experimental values taken from the literature for (a) Indium samples, (b) Gold samples, (c) Cobalt samples, (d) Copper samples, (e) Iron samples and (f) Indium, Gold, Cobalt, copper and Iron samples. Experimental data were those of Mahmoud et al [29], Taylor and Linacre [30], Carre et al [31], Hasnain et al [32], Sola [33], Walker et al [34], Klema [35], and Crane and Doerner [36] as adopted from Martinho et al [22]. The uncertainty of $G_{\text{th}}$ was added as 10% for all experimental values of $G_{\text{th}}$ due to digitization uncertainty. (F: Foil, C: Cylinder, W: Wire, and G: General Convex body, our approach). Error bars are either the digitization errors or a given uncertainty, see section 2.

Figure 2. Comparison of $G_{\text{th}}$ of our approach with Experimental values taken from the literature for (a) Indium samples, (b) Gold samples, (c) Cobalt samples, (d) Copper samples, (e) Iron samples and (f) Indium, Gold, Cobalt, copper and Iron samples.
Elements were Au, Co, Mn and Na in the form of wires, foils or in finite slabs. Note that our model calculations were based on the derived formula in equation (14) and the interaction probability in equation (43). Conducting experiments on infinite foils or wires are not feasible experimentally. Most probably, the researchers had conducted their experiments on finite wire where the ratio between the radius and the height approached zero; similarly, they may have conducted their experiments on finite foils where the ratios between thickness and other dimensions are very small. Parameters such as foil thickness, wire radius and cylinder height were obtained from the original sources of the experimental data, but there was no information on the limitations of the infinite dimension axis. It is worth mentioning that such a finite-dimensional size increases the value of the experimentally measured self-shielding factor and may cause discrepancies among results with different sample conditions. Hence, the experimental bias in the

Figure 3. Comparison of $G_{ep}$ of our derived formula, as in equation (14) using the interaction probability of equation (43), for (a) and (b) Gold samples, (c) Manganese samples, (d) Cobalt samples, (e) Sodium samples and (f) Gold, Cobalt, Manganese and Sodium samples with experimental values taken from Gonalves et al [19], Lopes [38, 39], McGarry [40], Brose [41], Yamamoto et al [42], Jefferies et al [43], Eastwood and Werner [37], and Kumpf [44]. (F: Foil, W: Wire, S: Infinite Slab, and G: General Convex body, our approach). Error bars are either given or due to digitization, see section 2.

Gonalves et al [19], Lopes [38, 39], McGarry [40], Brose [41], Yamamoto et al [42], Jefferies et al [43], Eastwood & Werner [37], and Kumpf [44] were used for comparison. Elements were Au, Co, Mn and Na in the form of wires, foils or infinite slabs. Note that our model calculations were based on the derived formula in equation (14) and the interaction probability in equation (43). Conducting experiments on infinite foils or wires are not feasible experimentally. Most probably, the researchers had conducted their experiments on finite wire where the ratio between the radius and the height approached zero; similarly, they may have conducted their experiments on finite foils where the ratios between thickness and other dimensions are very small. Parameters such as foil thickness, wire radius and cylinder height were obtained from the original sources of the experimental data, but there was no information on the limitations of the infinite dimension axis. It is worth mentioning that such a finite-dimensional size increases the value of the experimentally measured self-shielding factor and may cause discrepancies among results with different sample conditions. Hence, the experimental bias in the
measurements made on infinite wire or foils is the main source of deviations between the present analytical formulae and the experimental results. With the adaptation in equation (44), our model gave a good representation of the experimental data for Au, Co, Mn and Na within the experimental uncertainty. Otherwise, the model curve shall be more steeper and mess up the experimental data. As shown in figure 2 and 3, there is a slight difference between the experimental, calculated values and our model in gold and indium wires and foils. The supplementary materials demonstrate how the formulae are used with numerical examples of gold having different geometries.

It is clear that the physics behind the neutrons’ self-shielding factor depends not only on the properties and geometry of the material but also on the neutron energy range as shown in figures 2 and 3. A comparison between the present approach of ab initio calculations, considering the extreme cases of infinite wire and infinite foil, and the empirical equation given in [19–23] are given in appendix D of the present work.

4. Conclusion

In the vicinity of neutron-absorbing elements within the sample, neutron flux shall be modified continuously with depth. The activation formulae that take the flux as a constant value shall be corrected by the corresponding self-shielding factor. This ab initio neutron self-shielding factor formula can be used for any other neutron fields, provided that the field is isotropic, the integral parameters of the material placed in such field are known, and the neutron field is neither varying nor oscillating in a manner that causes a difference in energy distribution over time. The mathematical formulae showed complete agreement with experimental results that assume Maxwellian energy distribution and, in principle, explained the discrepancy among the experimental measurements, especially those related to presumed infinite samples. The self-shielding corrected neutron flux factor, often obtained from numerous empirical approaches based on fitting, now can be calculated using the analytic formulae as presented in the present work. Understanding the physics behind self-shielding enabled the extension of a simple thermal neutron picture into the epithermal energies, with the possibility for application to high-energy neutrons. The analytical formulae enable its implantation the long-term application in the analysis of neutron activation and neutron-induced effects in materials in different geometries, especially neutron shields, using integral parameter representation, instead of a numeric one.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflict of interest

The authors declare that they have no known source for conflict of interest with any person.

Author contribution statement

The Author Contribution based on CRedit (Contributor Roles Taxonomy) is as follow:
Elsayed K Elmaghraby: Conceptualization, Data Curation, Writing—Original Draft.
Ateia W Mahmoud: Validation, Formal analysis, Investigation, Visualization.
E Salama: Methodology, Software, Writing—Review & Editing, Supervision.
A Elghazaly: Resources, Supervision.
S A El-fiki: Conceptualization, Writing—Review & Editing, Supervision.

Appendix A. Advantage compared to Monté Carlo methods

The use of Monté Carlo simulation software (MC) for calculating the self-shielding factors is feasible but not yet efficacious. The principle underlying MC is to avoid the direct analytical solution of the problem. The goal of MC is to simulate and average a sufficiently large number of particle histories to obtain estimates of the flux which include rigorous approximations. According to Larson, MC of difficult problems are often very costly to set up and run. To make the MC code run with acceptable efficiency, the code users must specify a large number of biasing parameters, which are specialized to each different problem. Determining these parameters can be difficult and time-consuming. Also, even when the biasing parameters are well-chosen, MC converges slowly and non-monotonically with increasing run time. Thus, while MC solutions are free of truncation errors, they
are certainly not free of statistical errors, and it is challenging to obtain MC solutions with sufficiently small statistical errors, and with acceptable cost. Finally, the non-analog techniques that have been developed for making MC simulations acceptably efficient and were useful for source-detector problems in which a detector response in a small portion of phase space is desired are not useful for obtaining efficient global solutions, over all of phase space. Generally, MC solutions work best when very limited information about the flux (e.g. a single detector response) is desired in a given simulation. MC is feasible for calculating the self-shielding of a single sample, it requires time and an experienced user to make the acceptable accuracy and efficiency, the expense most scientists cannot afford to just calculate a single parameter in their routine work. For example, considering a set of different samples need to be analyzed using neutron activation for the purpose of elemental analysis, MC SIM needs experience and a lot of time to reduce fluctuation, adopt the geometry, consideration of the neutron transport inside and outside the sample, and the absorption and scattering phenomenon as a function of neutron energy.

Although our intention while deriving and validating the present mathematical formulae was focused on avoiding such costs and enhancing present existing empirical equations and transforming all the problems from the spectroscopic set of parameters, such as thermal cross-section, thickness, width, height, radius, shape, a width of neutron first resonance, the width of the first gamma resonance, etc into an integrated set of well-known parameters, thermal cross-section, resonance integral, average chord length. All remaining factors are calculated from these three parameters. Of course, the thermal cross-section and sample mass and composition are common.

Appendix B. Contribution of velocity distribution

According to the results of Blaauw [18], the calculation of the reaction rate needs to be with neutron density averaged macroscopic cross-section (function of velocity) instead of flux averaged macroscopic cross-section (energy-dependent). Blaauw found that the self-shielding factors calculated for monoenergetic neutrons yield the same results as if they are used with the flux averaged macroscopic cross-section provided that the neutron density averaged macroscopic cross-section given by

$$\langle \Sigma \rangle = \frac{2}{\sqrt{\pi}} \frac{\Gamma_o}{T} \Sigma_o,$$  \hspace{1cm} (B.1)

is used instead of the flux averaged capture cross-section given by

$$\langle \Sigma \rangle = \frac{\sqrt{\pi}}{2} \frac{\Gamma_o}{T} \Sigma_o.$$  \hspace{1cm} (B.2)

Blaauw [18] results showed that the volume-averaged attenuation self-shielding factor in extended neutron distributions has an extra term that depends on the statistical moments of deviation in reciprocal velocity average. The contribution of this extra factor had been estimated by Goncalves et al [23] to be around $6 \pm 1\%$.

The higher order terms in equation (9) (Denoted $\mathcal{R}$ ) can be obtained from Blaauw [18] and adapted to our notions as;

$$\mathcal{R} \cong \sum_{i=1}^{\infty} \frac{(-1)^i}{i!} (\Sigma_o)^{v_t} \left( \left\langle \frac{1}{v} \right\rangle - \left\langle \frac{1}{v^2} \right\rangle \right) \int_v (\vec{r})^i d\vec{r}$$  \hspace{1cm} (B.3)

For the first term, $i = 1$, the value of $\left\langle \frac{1}{v} \right\rangle - \left\langle \frac{1}{v^2} \right\rangle$ vanishes. While for approximate spherical symmetry the integral yields the average squared length over the volume of the sphere, The first term comprises;

$$\int_v (\vec{r})^2 d\vec{r} = \int_0^\pi \int_0^{2\pi} \int_0^\pi r^2 (r \sin \phi) d\phi dr d\phi$$  \hspace{1cm} (B.4)

$$\frac{4}{5} \pi r^5 = \frac{4}{5} \pi r^5 r^2 \frac{3}{5} = \frac{3}{5} r^2$$  \hspace{1cm} (B.5)

For the first approximation, only the term of $i = 2$ has an effective contribution. Hence,

$$\mathcal{R} \cong \frac{+1}{2} (\Sigma_o)^{v_t} \left( \left\langle \frac{1}{v^3} \right\rangle - \left\langle \frac{1}{v^4} \right\rangle \right) \frac{3}{5} r^2$$  \hspace{1cm} (B.6)

For Maxwellian velocity distribution

$$\left\langle \frac{1}{v} \right\rangle = \frac{2}{\sqrt{\pi}} \frac{1}{v_o}$$  \hspace{1cm} (B.7)
\[ \left\langle \frac{1}{v^2} \right\rangle = 2 \frac{1}{v_0^2} \]  \hspace{1cm} (B.8)

\[ \mathcal{R} \approx (\Sigma_a \bar{E}) \frac{3}{5} \left( 1 - \frac{2}{\pi} \right) \approx 0.218 (\Sigma_a \bar{E})^2, \text{ Maxwellian} \]

\[ \approx 0, \text{ monoenergetic} \]

\[ \approx 0, \quad 20 v_0 \leq v \leq 4 \times 10^5 v_0 \]  \hspace{1cm} (B.9)

The first formula is valid only for the entire range of Maxwellian neutron distribution. However, for practical use, only the epithermal range between cadmium cutoff at 0.5 eV about 1 MeV is used. In such cases, the difference \( \left( \left\langle \frac{1}{v^2} \right\rangle - \left\langle \frac{x^2}{v^2} \right\rangle \right) \) practically vanishes, \( \mathcal{R} \approx 0 \).

There is an additional reason why this value is ignored within the sample in the present work. The Blaauw [18] derivation is based on the idea that the neutron flux distribution has a constant shape as it passes through the depth \( \bar{E} \). However, there is a simple experimental remark in neutron physics: whenever the neutron energy distribution repudiates the proper thermalization distribution (Maxwellian + 1/E dependence in epithermal region) by any mean such as absorption, the neutrons rapidly redistribute its velocity population within the diffusion distance to follow the proper distribution—up to thermalization. The idea is, that even if there is the absorption of neutrons having a velocity \( v \) in equation (B.3) at some distance, there was a sort of recovery of that distribution. And hence, the difference in equation (B.6) has much less value than expected by Blaauw.

**Appendix C. Determination of chord lengths based on neutron transport formulae**

The time dependent diffusion equation comprises;

\[
\frac{1}{v_{av}} \frac{\partial \varphi(\vec{r}, t)}{\partial t} = \nabla \cdot J(\vec{r}, t) - \Sigma_a \varphi(\vec{r}, t) + Q(\vec{r}, t),
\]  \hspace{1cm} (C.1)

where \( J(\vec{r}, t) = D(\vec{r}, t) \nabla \varphi(\vec{r}, t) \) is the neutron current, \( Q(\vec{r}, t) \) is the neutron production rate within the medium in units of \( n \text{ cm}^{-3}\text{s}^{-1} \). Under the condition of steady-state \( \frac{\partial \varphi(\vec{r}, t)}{\partial t} = 0 \) and considering:

- the sample is embedded within a uniform neutron field in which the flux outside it, \( \varphi_{\infty} \), to be isotropic, and uniform and does not depend on the diffusion within the sample,
- our situation of the sample absorbing neutrons not generating it,

the solution of the problem comes as **difference-problem** in the steady-state where \( Q(\vec{r}, t) \) equated to \( \varphi_{\infty} \), and considering only the difference replacing \( \varphi(\vec{r}) \) by \( \varphi_x - \phi(\vec{r}) \): Then

\[
\nabla \cdot D(\vec{r}) \nabla \phi(\vec{r}) - \Sigma_a(\vec{r}) \phi(\vec{r}) = 0
\]  \hspace{1cm} (C.2)

In the homogenous isotropic medium, \( D(\vec{r}) \) and \( \Sigma_a(\vec{r}) \) are constants.

\[
\nabla^2 \phi(\vec{r}) - B^2 \phi(\vec{r}) = 0,
\]  \hspace{1cm} (C.3)

The \( B \) factor is the geometric buckling factor in reactor physics. Taking into consideration that \( \Sigma_a = 1/\lambda_a \) and \( D = \lambda_s/3 \) where \( \lambda_s \) is the absorption mean-free path and \( \lambda_s \) is the transport scattering diffusion length given by the more advanced transport theory in terms of transport and absorption cross-sections equation as [74, 75];

\[
\lambda_s = \frac{1}{\Sigma_a + \Sigma(1 - \bar{\mu})},
\]  \hspace{1cm} (C.4)

where \( \bar{\mu} = \frac{2}{3} \) is average value of the cosine of the angle in the lab system. So,

\[
B^2 = \frac{\Sigma_a [\text{cm}^{-1}]}{D[\text{cm s}^{-1}]}.
\]  \hspace{1cm} (C.5)

**C.1. Rectangular geometries**

In cartesian coordinates, equation (C.3) is reduced to three independent equations by the separation of variables assuming \( \phi(\vec{x}, \vec{y}, \vec{z}) = \phi_x(\vec{x}) \phi_y(\vec{y}) \phi_z(\vec{z}) \). I.e.

\[
\left( \frac{d^2}{dx^2} - B_x^2 \right) \phi_x(\vec{x}) = 0
\]  \hspace{1cm} (C.6)
The general solution is:
\[ \phi(x, y, z) = \text{Const.} e^{-\text{i}b_1 x} e^{-\text{i}b_2 y} e^{-\text{i}b_3 z} \]  
\[ (C.9) \]

7. Cylindrical geometries

For a definite convex shape having cylindrical geometries, equation (C.3) becomes the Helmholtz differential equation;
\[ \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} + B^2 \right) \phi(\rho, \phi, z) = 0. \]  
\[ (C.10) \]

In which the metric tensor scale factors are \( 1, \rho, \) and \( 1 \) for the coordinates \( \rho, \phi, z, \) respectively. Separation of variables is done by writing
\[ \phi(\rho, \phi, z) = \phi_\rho(\rho) \phi_\phi(\phi) \phi_z(z). \]  
\[ (C.11) \]

The solutions are
\[ \phi_\rho(\rho) = C_4 \cos m \phi + C_5 \sin m \phi, \]  
\[ (C.13) \]
\[ \phi_\phi(\phi) = C_7 \cos m \phi + C_8 \sin m \phi, \]  
\[ (C.14) \]
\[ \phi_z(z) = C_9 e^{-\sqrt{n^2-B_1^2} z} + C_4 e^{\sqrt{n^2-B_1^2} z} \]  
\[ (C.18) \]
\[ \phi_\rho(\rho) = C_7 J_n(\sqrt{n^2+B_1^2} \rho) + C_8 Y_n(\sqrt{n^2+B_1^2} \rho), \]  
\[ (C.20) \]

where \( J_n \) and \( Y_n \) are Bessel functions of the first kind and second kind, respectively. These results require that \( n \) and \( m \) be integers. \( Y_\rho(0) = -\infty \) which leads to an un-physical solution, hence, \( C_2 = 0 \) and \( C_8 = 0. \) Similarly, \( C_4 = 0 \) and \( C_6. \) The solution is reduced to;
\[ \phi(\rho, \phi, z) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_{mn} I_m(\sqrt{n^2 + B_1^2 \rho}) \cos m \phi \]
\[ e^{-\sqrt{n^2 - B_z^2} z} \text{ if } n^2 > B_z^2 \]
\[ = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_{mn} I_m(\sqrt{n^2 + B_1^2 \rho}) \cos m \phi \cos \sqrt{B_z^2 - n^2 z} \text{ if } n^2 \leq B_z^2 \]

where \( C_{mn} \) is a constant that depends on the values of \( m \) and \( n \).

C.3. Spherical geometries
In spherical coordinates, equation (C.3) resembles;
\[ \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \phi + B_1^2 \phi = 0. \]

Because of the spherical symmetry there is only one value of \( B = B_1 \). Values of \( B_2 \) and \( B_3 \) vanishes; i.e. \( \ell_2 = \infty \) and \( \ell_3 = \infty \).
\[ \left( \frac{1}{r} \frac{d}{dr} \left( r \frac{d}{dr} \right) + \frac{1}{\cos \theta} \frac{d}{d\theta} \left( \cos \theta \frac{d}{d\theta} \right) + \frac{1}{\sin^2 \theta} \frac{d^2}{d\phi^2} \right) \phi + B_1^2 \phi = 0. \]

Separation of variable requires substitution of \( \phi(r, \theta, \phi) \) by \( \phi_{\ell}(r) \phi_{\theta}(\theta) \phi_{\phi}(\phi) \). Separating the \( r \) term with separation constant \( \ell(l+1) \)
\[ \frac{1}{\phi_{\ell}} \frac{d}{dr} \left( r \frac{d\phi_{\ell}}{dr} \right) - l(l+1) + r^2 B_1^2 = 0 \]
\[ \frac{1}{\phi_{\theta}} \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\phi_{\theta}}{d\theta} \right) + \frac{1}{\phi_{\phi}} \frac{1}{\sin^2 \theta} \frac{d^2\phi_{\phi}}{d\phi^2} + l(l+1) = 0 \]

Equation (C.26) is separated by separation constant \( m^2 \), then
\[ \frac{1}{\phi_{\theta}} \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\phi_{\theta}}{d\theta} \right) + l(l+1) \sin \theta - m^2 = 0 \]
\[ \frac{1}{\phi_{\phi}} \frac{d^2\phi_{\phi}}{d\phi^2} + m^2 = 0 \]

solution of equations (C.25), (C.27), and (C.28) yield the following solution;
\[ \phi(r, \theta, \phi) = \sum_{L=0}^{\infty} \sum_{m=0}^{\infty} C_{mn} j_1(B_1 r) P_m^L(\cos \theta) \cos m \phi \]

by ignoring the anti symmetric terms Here, \( P_m^L(\cos \theta) \) gives the associated Legendre polynomial while \( j_1(B_1 r) \) is the spherical Bessel function.

Appendix D. Comparison with empirical formula

Figures D.1 and D.2 represent the thermal self-shielding factor calculated using empirical equations given by [19–23].

Their curves were calculated with the specific values of cross-sections given in their manuscripts, which are not equal to the recommended cross-sections in literature. Our approach was calculated using the extreme approximation of infinite foil (having only one variable which is the thickness) and with the general cross-section values in [10, 54, 55]. Based on this comparison based on extreme cases of infinite wire and infinite foil, the results of our approach matched the empirical equation in most cases, where it had already succeeded. Note that: there is no such infinite foil or infinite wire in experimental situations.
Figure D.1. A comparison between the present general approach of \textit{ab initio} calculations, considering the extreme cases of infinite wire, and the empirical equation given in [19–23]. Experimental data from Taylor and Linacre [30], Carre et al [31], were digitized from Martinho et al [22]. While the data of Eastwood and Werner [37] for Co Wire was collected from their original values.

Figure D.2. A comparison between the present approach of \textit{ab initio} calculations, considering the extreme cases of infinite foil, and the empirical equation given in [19–23]. Experimental data from Hasnain \textit{et al} [32], Sola [33], Walker \textit{et al} [34], Klema [35], and Crane and Doerner [36] were digitized from Martinho \textit{et al} [22].

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