



A Conventional Phase Function with the Chebyshev Polynomials of Second Kind for the Criticality Problem in Transport Theory

Hakan ÖZTÜRK

*Osmaniye Korkut Ata University, Faculty of Arts and Sciences, Department of Physics, 80000 Osmaniye, Türkiye,
hakanozturk@osmaniye.edu.tr*

Abstract

The criticality calculations for one-speed neutrons in a finite homogenous slab are done using the conventional Henyey-Greenstein (HG) phase function in transport theory. After defining the phase function in transport equation, the neutron angular flux is expanded in terms of the Chebyshev polynomials of second kind (U_N method). Then, the critical half-thicknesses of the slab are calculated for various values of the scattering parameters. The numerical results obtained from the present method are given in the tables together with the ones obtained using an alternative phase function (Anlı-Güngör, AG) for comparison.

Keywords: Henyey-Greenstein Function, Critical Slab, U_N Method, Transport Equation.

Transport Teoride Kritiklik Problemi için İkinci Tip Chebyshev Polinomları ile Konvansiyonel Bir Faz Fonksiyonu

Özet

Transport teoride konvansiyonel Henyey-Greenstein (HG) faz fonksiyonu kullanılarak sonlu homojen bir dilimdeki nötronlar için kritiklik hesaplamaları

yapılmıştır. Transport denkleminde faz fonksiyonu tanımlandıktan sonra, açılmal n6tron akısı ikinci tip Chebyshev polinomları cinsinden seriye aılmıştır (U_N metodu). Daha sonra, saılma parametrelerinin farklı deęerleri iin dilimin yarı-kalınlıkları hesaplanmıřtır. Mevcut metotla elde edilen n6merik sonular, alternatif faz fonksiyonu (Anlı-G6ng6r, AG) kullanılarak elde edilen sonular ile karřılařtırma yapmak iin tablolarda verilmiřtir.

Anahtar Kelimeler: Henyey-Greenstein Fonksiyonu, Kritik Dilim, U_N Metodu, Transport Denklemi.

1. Introduction

The particle or Boltzmann transport equation explains the interactions and the conservation of the number of neutrons in a system. It is important to know the types of interactions and then the number of neutrons in a fission reactor to continue the fission chain reaction and to control that reactor. Therefore, the investigation of the criticality of a reactor is one of the main problems of neutron transport theory.

There are many methods for the solution of the transport equation in literature. Among them, the discrete ordinates and the polynomials expansion based techniques are most common and powerful ones [1-4]. However in some cases, an approximation related with the scattering function or the neutron angular flux can take the problem away from the realism. Therefore, exact scattering models are preferred to use in scattering function in order to approach the real system better [1,2].

One of the first attempts developed for the scattering function even for particles or waves belongs to Henyey and Greenstein (HG) [5]. This HG phase function was used in radiative transfer equation in their studies and then this function was used in other studies by the researchers [6-8].

In this paper, the conventional HG phase function is used for the scattering function in transport equation. Then, the resultant transport equation is solved for the criticality problem in slab geometry. The neutron angular flux is expanded in terms of the Chebyshev polynomials of second kind (U_N method) which was successfully applied to the problems of transport theory before [9,10]. After deriving the moment equations, the criticality equation is obtained for one-speed neutrons in a finite

homogeneous slab of thickness $2a$ extending from $-a$ to a . Finally, the critical half-thicknesses of the slab are calculated for certain scattering parameters and various collision parameters. The calculated results for the critical half-thicknesses obtained from the present method with an increasing order of the U_N approximation with the ones obtained from the alternative phase function (AG) are listed in the tables for comparison [11,12].

2. U_N Method for the Transport Equation with Henyey-Greenstein Phase Function

The neutron transport equation for one-speed neutrons in a source free medium can be written in conservative form,

$$\mathbf{\Omega} \cdot \nabla \psi(r, \mathbf{\Omega}) + \sigma_T \psi(r, \mathbf{\Omega}) = \int_{\mathbf{\Omega}'} \psi(r, \mathbf{\Omega}') \sigma_s(\mathbf{\Omega}' \cdot \mathbf{\Omega}) d\mathbf{\Omega}', \quad (1)$$

where $\mathbf{\Omega}'$ is the unit vector of neutron velocity before (and $\mathbf{\Omega}$ after) a scattering collision, c is the cross-section parameter; number of secondary neutrons per collision and σ_T is the total macroscopic cross-section. $\psi(r, \mathbf{\Omega})$ is the neutron angular flux at position r in direction $\mathbf{\Omega}$ and $\sigma_s(\mathbf{\Omega} \cdot \mathbf{\Omega}')$ is the scattering function [1].

In this work, the neutron angular flux is expanded in terms of the Chebyshev polynomials of second kind and the HG phase function is used as a scattering function in one-speed transport equation to calculate the critical half-thickness of the homogeneous slab for various values of the scattering parameters.

The HG phase function can be written as [5],

$$\sigma_s^{HG}(\mu_0) = \frac{\sigma_s(1-t^2)}{4\pi(1-2\mu_0 t + t^2)^{3/2}}, \quad (2)$$

where σ_s is any non-negative coefficient, t is the parameter representing all kind of scattering (forward, backward and anisotropic, etc.) in the range of $-1 \leq t \leq 1$, and $\mu_0 = \mathbf{\Omega} \cdot \mathbf{\Omega}'$ is the cosine of the scattering angle [5],

$$\mu_0 = \mu\mu' + \sqrt{1-\mu^2}\sqrt{1-\mu'^2} \cos(\varphi - \varphi'). \quad (3)$$

As an indicator of the U_N method, neutron angular flux is expanded in terms of the Chebyshev polynomials of second kind [9,10],

$$\psi(x, \mu) = \frac{2}{\pi} \sqrt{1-\mu^2} \sum_{n=0}^N \Phi_n(x) U_n(\mu), \quad -a \leq x \leq a, \quad -1 \leq \mu \leq 1. \quad (4)$$

The steady state transport form of Eq. (1) for one-dimensional case can be written when Eq. (2) is inserted on the right hand side of Eq. (1),

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \sigma_T \psi(x, \mu) = \int_{-1}^1 \psi(x, \mu') d\mu' \int_0^{2\pi} \frac{\sigma_s(1-t^2)}{4\pi(1-2\mu_0 t + t^2)^{3/2}} d\varphi', \quad (5)$$

subject to free space boundary and symmetry conditions:

$$\psi(a, \mu) = 0, \quad (6a)$$

$$\psi(x, \mu) = \psi(-x, \mu), \quad \mu > 0. \quad (6b)$$

By means of the addition theorem of the Legendre polynomials ($P_n(\mu)$), the integrand on the right hand side of Eq. (5) over $d\varphi'$ can be obtained as [13],

$$\int_0^{2\pi} \frac{\sigma_s(1-t^2)}{4\pi(1-2\mu_0 t + t^2)^{3/2}} d\varphi' = \frac{\sigma_s}{2} \sum_{n=0}^{\infty} (2n+1) t^n P_n(\mu) P_n(\mu'). \quad (7)$$

Then, one-dimensional transport equation can be written using Eq. (7) in Eq. (5),

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \nu \psi(x, \mu) = \frac{\nu c}{2} \sum_{n=0}^{\infty} (2n+1) t^n P_n(\mu) \Phi_n(x), \quad (8)$$

where $c = \sigma_s / \sigma_T$, the number of secondary neutrons per collision. A dimensionless space variable such that $\sigma_T x / \nu \rightarrow x$ is defined in order to simplify the derivation of the equations and ν is the eigenvalues.

In solution procedure of the method, the orthogonality and the recurrence relations of the Chebyshev polynomials of second kind are needed and thus they are given as respectively [14],

$$\int_{-1}^1 U_n(\mu) U_m(\mu) \sqrt{1-\mu^2} d\mu = \frac{\pi}{2} \delta_{n,m}, \quad (9)$$

$$U_{n+1}(\mu) - 2\mu U_n(\mu) + U_{n-1}(\mu) = 0. \quad (10)$$

Then, the neutron angular flux $\psi(x, \mu)$ given in Eq. (4) is inserted into Eq. (8), and then the resulting equation is multiplied by $U_m(\mu)$ and integrated over the definition of the $\mu \in (-1,1)$. A general expression for the U_N moments of the angular flux could not be obtained in this study, but instead individual expressions as an example for $n = 0,1,2$ can be written as,

$$\frac{d\Phi_1(x)}{dx} + 2\nu \Phi_0(x) = 2\nu c \Phi_0(x), \quad (11a)$$

$$\frac{d\Phi_2(x)}{dx} + \frac{d\Phi_0(x)}{dx} + 2\nu \Phi_1(x) = 2\nu c t \Phi_1(x), \quad (11b)$$

$$\frac{d\Phi_3(x)}{dx} + \frac{d\Phi_1(x)}{dx} + 2\nu \Phi_2(x) = -2\nu c \left\{ \frac{1}{3} (t^2 - 1) \Phi_0(x) - t^2 \Phi_2(x) \right\}, \quad (11c)$$

where $\Phi_{-1}(x) = 0$. When a well-known solution of the form [1],

$$\Phi_n(x) = A_n(\nu, t) \exp(x), \quad (12)$$

is used in Eq. (11), analytic expressions for all $A_n(\nu)$'s can be obtained as follows,

$$A_1(\nu, t) + 2\nu A_0(\nu, t) = 2\nu c A_0(\nu, t), \quad (13a)$$

$$A_2(\nu, t) + A_0(\nu, t) + 2\nu A_1(\nu, t) = 2\nu c t A_1(\nu, t), \quad (13b)$$

$$\frac{2}{3}\nu c(t^2 - 1)A_0(\nu, t) + A_1(\nu, t) + 2\nu(1 - ct^2)A_2(\nu, t) + A_3(\nu, t) = 0, \quad (13c)$$

where $A_{-1}(\nu, t) = 0$ and $A_0(\nu, t) = 1$. In order to simplify the solutions in the case of higher order approximations, Eq. (13) can also be written in a matrix form,

$$[M(\nu)]A(\nu, t) = 0, \quad (14)$$

where $M(\nu)$ is the $(N + 1) \times (N + 1)$ coefficient matrix and $A(\nu, t) = [A_0, A_1, \dots, A_N]^T$. One can obtain non-trivial solutions for the discrete eigenvalues by equating the determinant of the coefficient matrix to zero, i.e. $\det[M(\nu)] = 0$.

In U_N method, as in traditional Legendre polynomials approximation (P_N method), the discrete and continuum ν eigenvalues can be obtained by setting $A_{N+1}(\nu, t) = 0$ for various values of c and t . As an example for U_1 approximation, the coupled equations (13a and b) are solved together and an analytic expression for the eigenvalues are derived by setting $A_2(\nu, t) = 0$ in these equations,

$$\nu_k = \pm \frac{1}{2\sqrt{(1-c)(1-ct)}}. \quad (15)$$

In a similar manner, the determinant of a 2×2 matrix is equated to zero and then one can obtain the same result as in Eq. (15).

After the discrete eigenvalues ν_k for $k = 1, \dots, N + 1$ are computed, the general solution of the flux moments for odd numbers of N , i.e. Eq. (12) can be written as,

$$\Phi_n(x) = \sum_{k=1}^{(N+1)/2} \alpha_k A_n(v_k, t) \left[\exp\left(\frac{\sigma_T x}{v_k}\right) + (-1)^n \exp\left(-\frac{\sigma_T x}{v_k}\right) \right], \quad (16)$$

where the coefficients α_k can be determined from the physical boundary conditions of the system, and the parity relation of $A_n(-v, t) = (-1)^n A_n(v, t)$ is used. Eq. (16) can be interpreted as the summation of eigenvectors corresponding to each eigenvalues and it can also be represented as a general solution of the problem.

3. Boundary Conditions and the Criticality Problem

Determination of the eigenvalues is accepted to be equal to the problem of critical size of the system under consideration in neutron transport theory. Therefore, it is important to compute the eigenvalues and then the corresponding eigenfunctions in the problems of neutron transport.

Although the P_N approximation is one of the most powerful and the common methods used in the solution of the problems of photon and particle transport, it is a rather poor representation of the angular flux near material boundaries in slab geometries. Mark and Marshak vacuum boundary conditions are frequently used for the criticality problems. However, the Marshak boundary condition which is based on the condition of zero incoming current at the vacuum boundary is somewhat more accurate than the Mark condition, at least for small N [3,15]. Therefore in this study, the Marshak boundary condition is preferred for the calculation of the critical half-thickness of the slab. It can be written for U_N approximation of odd order,

$$\int_0^1 \psi(a, -\mu) U_k(-\mu) d\mu = 0, \quad k = 1, \dots, N. \quad (17)$$

First Eq. (16) is inserted into Eq. (4) and then the resulting equation of angular flux is written in Eq. (17) with the parity relation of the Chebyshev polynomials of second kind $U_k(-\mu) = (-1)^k U_k(\mu)$, one can obtain the criticality condition,

$$\frac{2}{\pi} \sum_{n=0}^N (-1)^{n+k} \left\{ \sum_{k=1}^{(N+1)/2} \alpha_k A_n(\nu_k, t) \left[\exp\left(\frac{\sigma_T a}{\nu_k}\right) + (-1)^n \exp\left(-\frac{\sigma_T a}{\nu_k}\right) \right] \right\} I_{n,k} = 0, \quad (18)$$

where $I_{n,k}$ is given by,

$$I_{n,k} = \int_0^1 U_n(\mu) U_k(\mu) \sqrt{1-\mu^2} d\mu = \begin{cases} \pi/4, & n=k, \\ \frac{\sin[(n-k)\pi/2]}{2(n-k)} + \frac{\sin[(n+k)\pi/2]}{2(n+k+2)}, & n \neq k, \end{cases} \quad (19)$$

and

$$\int_0^1 U_n(-\mu) U_k(-\mu) \sqrt{1-\mu^2} d\mu = (-1)^{n+k} I_{n,k}. \quad (20)$$

Eq. (18) can also be written in a matrix notation,

$$\left[M_m^k(a) \right] \beta_k = 0, \quad m, k = 1, 2, \dots, (N+1)/2, \quad (21)$$

where β_k is the column vector with elements of $[\beta_1, \beta_2, \dots, \beta_{(N+1)/2}]^T$ and $M_m^k(a)$ is the coefficient matrix with $(N+1)/2 \times (N+1)/2$ elements. For a non-trivial solution of Eq. (18) or (21), the coefficients β_k should be nonzero or the determinant of the coefficient matrix must vanish, i.e. $\det[M_m^k(a)] = 0$. As an example, it is easy to find an analytic solution for the critical half-thickness of the slab by setting $N = 1$ in Eq. (18) or Eq. (21) together with the eigenvalues which is already derived for U_1 approximation in Eq. (15),

$$a = \frac{1}{2\sigma_T \sqrt{(1-c)(1-ct)}} \tanh^{-1} \left(-\frac{8}{3\pi} \sqrt{\frac{(1-ct)}{(1-c)}} \right). \quad (22)$$

4. Numerical Results

The U_N method, i.e. the expansion of the neutron angular flux in terms of the Chebyshev polynomials of second kind, is applied to one-speed neutron transport equation for the critical slab problem using the Marshak boundary condition. The conventional HG phase function, a direct scattering function instead of an approximation, is used as the scattering function presented in transport equation and this direct selection and such searches are very important for the accurate solution of the transport equation now and later. Various orders of U_N approximation are used for the numerical solutions of the critical half-thickness of the slab and the results obtained from the present method for different values of c and t are tabulated in Tables 1 and 2. Additionally, the results obtained from the conventional P_N method and the ones obtained by Öztürk and Ege are given in the same tables for comparison [12,16]. The total macroscopic cross section is taken as to be its normalized value, $\sigma_T = 1 \text{ cm}^{-1}$ and all computations are carried out using Maple software.

In this study, first the HG phase function is used instead of the neutron scattering function after taking the transport equation in slab geometry. Then, the neutron angular flux is expanded in terms of the Chebyshev polynomials of second kind as successfully applied to the problems in transport theory in the last decade [9,10]. And U_N moments of the angular flux are obtained. A well-known solution of the form of Eq. (12) is replaced to moment equations to obtain the discrete eigenvalues by setting $A_{N+1}(\nu) = 0$ for various values of c and t . Finally, the criticality equation (Eq. (12)) is obtained using the Marshak boundary condition. And so the critical half-thicknesses of the slab are computed for $N = 1, 5$ and 9 order approximations for various values of c and t and they are given in the tables.

In Tables 1 and 2, the critical half-thicknesses of the slab are listed for the most common values of $c = 1.20$ and 2.00 with an increasing order of t from -1 to 1 . $t = 0$ case can be tested as corresponding to isotropic scattering [13].

Table 1. Critical half-thicknesses for $c = 1.20$ as calculated by various orders of U_N approximation

t	U_1 (cm)	U_5 (cm)	U_9 (cm)	P_9 [11] (cm)	Ref. [16] (cm)
-1	0.92676	1.73300	0.93212	0.82263	1.13597
-3/4	0.97796	0.94280	0.94459	0.94540	1.17679
-1/2	1.03956	1.08197	1.08505	1.08574	1.21505
-1/4	1.11584	1.18237	1.18514	1.18579	1.25241
0	1.21406	1.28759	1.28974	1.29038	1.28974
1/4	1.34808	1.41343	1.41468	1.41535	1.32763
1/2	1.54897	1.57200	1.57172	1.57247	1.36662
3/4	1.91122	1.73388	1.72714	1.72790	1.40719
1	3.12985	1.17848	0.72137 ^a	0.75727 ^a	1.44965

^aAll eigenvalues of the spectrum are real.**Table 2.** Critical half-thicknesses for $c = 2.00$ as calculated by various orders of U_N approximation

t	U_1 (cm)	U_5 (cm)	U_9 (cm)	P_9 [11] (cm)	Ref. [16] (cm)
-1	0.28103	0.52410	0.24435	0.25514	0.27071
-3/4	0.29423	0.21418	0.19727	0.19904	0.28734
-1/2	0.30979	0.26806	0.26085	0.26240	0.29832
-1/4	0.32856	0.29758	0.29236	0.29378	0.30651
0	0.35191	0.31826	0.31294	0.31418	0.31294
1/4	0.38224	0.33306	0.32598	0.32702	0.31793
1/2	-	-	-	-	0.32135
3/4	0.49036	0.30600	0.27057	0.27290	0.32260
1	0.62597	0.23570	0.14427	0.15146 ^a	0.32021

^aAll eigenvalues of the spectrum are real.

5. Conclusion

In this paper, the critical slab problem for one-speed neutrons is studied using U_N method. The conventional HG phase function is used for the scattering kernel in transport equation and the numerical results for the critical half-thickness of the slab are obtained for various values of c and t using different orders of the U_N approximation. While the positive values of t is referred to as the forward peaked scattering of the neutrons, the negative values of it is referred to as the backward peaked scattering of the neutrons. Both positive and negative values of the parameter t are used. Physically these are meaningful about the interaction of neutrons with the nuclei in the system [13].

It is seen from the numerical results given in the tables that the critical half-thickness of the slab increases with the increasing values of t and decreasing values of c . The behavior of the critical thickness is non-monotonic in the case of strongly forward

scattering when $c = 1.20$ and 2.00 . This non-monotonic behavior of the critical thickness is observed especially in higher order approximations. That is, the critical thickness repeats its non-monotonic behavior in the case of forward peaked scattering as reported before [17,18].

At the end, one can summarize from the equations flowing in this study that the HG phase function can be applied to photon or particle transport problems with simply derivable equations. It can also be applied to other problems including a phase function in science and engineering.

References

- [1] Davison, B., Neutron Transport Theory, Oxford University Press, London, 1958.
- [2] Case, K. M., Zweifel, P. F., Linear Transport Theory, Addison-Wesley Publishing Company, 1967.
- [3] Bell, G. I., Glasstone, S., Nuclear Reactor Theory, VNR Company, New York, 1972.
- [4] Sahni, D. C., Sjöstrand, N. G., Garis, N. S., *Criticality and time eigenvalues for one-speed neutrons in a slab with forward and backward scattering*, J. Phys. D: Appl. Phys., 25, 1381-1389, 1992.
- [5] Henyey, L. G., Greenstein, J. L., *Diffuse radiation in the galaxy*, Astrophys. J., 93, 70-83, 1941.
- [6] Reynolds, L. O., McCormick, N. J., *Approximate two parameter phase function for light scattering*, J. Op. Soc. Am., 70, 1206-1212, 1980.
- [7] Williams, M. M. R., *A synthetic scattering kernel for particle transport in absorbing media with anisotropic scattering*, J. Phys. D: Appl. Phys., 11, 2455-2463, 1978.
- [8] Liu, P., *A new phase function approximating to Mie scattering for radiative transport equations*, Phys. Med. Biol., 39, 1025-1036, 1994.
- [9] Öztürk, H., *The reflected critical slab problem for one-speed neutrons with strongly anisotropic scattering*, Kerntechnik, 73, 66-74, 2008.
- [10] Öztürk, H., Anlı, F., Güngör, S., *Application of the U_N method to the reflected critical slab problem for one-speed neutrons with forward and backward scattering*, Kerntechnik, 72, 74-76, 2007.

- [11] Öztürk, H., Anlı, F., *Diffusion approximation for certain scattering parameters of the Anlı-Güngör phase function*, Kerntechnik, 77, 381-384, 2012.
- [12] Öztürk, H., *Application of the Henyey-Greenstein and Anlı-Güngör phase functions for the solution of the neutron transport equation with Legendre polynomials: Reflected critical slab problem*, Kerntechnik, 78, 447-453, 2013.
- [13] Anlı, F., Yaşa, F., Güngör, S., *General eigenvalue spectrum in a one-dimensional slab geometry transport equation*, Nucl. Sci. Eng., 150, 72-77, 2005.
- [14] Arfken, G., *Mathematical Methods for Physicists*, Academic Press, Inc., London, 1985.
- [15] Lee, C. E., Dias, M. P., *Analytical solutions to the moment transport equations-I; one-group one-region slab and sphere criticality*, Ann. Nucl. Energy, 11, 515-530, 1984.
- [16] Öztürk, H., Ege, Ö., *An application of the alternative phase function with the second kind of Chebyshev polynomials: The criticality problem in transport theory* (submitted to Kerntechnik).
- [17] Yıldız, C., *Variation of the critical slab thickness with the degree of strongly anisotropic scattering in one-speed neutron transport theory*, Ann. Nucl. Energy, 25, 529-540, 1998.
- [18] Sahni, D. C., Sjöstrand, N. G., *Non-monotonic variation of the criticality factor with the degree of anisotropy in one-speed neutron transport*, Transp. Theory Statist. Phys., 20, 339-349, 1991.