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Calculation of Diffusion Coefficients using Modified UN Method with Anli-Güngör Scattering Function

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Research Article	**Abstract**
Received: 03.01.2022 Accepted: 27.06.2022 Published online: 30.06.2022	Modified U1 approximation applied to neutron transport equation and diffusion coefficients are calculated for certain values of scattering parameters (t) using Anli-Güngör scattering function. Analytical diffusion coefficient term is given and numerical results obtained from modified U1 and P1 approximations are compared with each other for different collision parameters and t parameters

Keywords: Modified U1 Approximation, Transport Equation, Anli-Güngör Scattering function, Diffusion length, Diffusion coefficient

Anli-Güngör Saçılma Fonksiyonu ile Modifiye UN Metodu Kullanılarak Difüzyon Katsayılarının Hesaplanması

Araştırma Makalesi	**Özet**
Geliş tarihi: 03.01.2022 Kabul tarihi:27.06.2022 Online Yayınlanma:30.06.2022	Modifiye U1 yaklaşımı nötron transport denklemine uygulandı ve Anli-Güngör saçılması kullanılarak saçılma parametresinin bazı değerleri için difüzyon katsayıları hesaplandı. Analitik difüzyon katsayısı terimi verildi ve Modifiye U1 ve P1 yaklaşımından elde edilen sayısal sonuçlar farklı çarpışma ve t parametreleri için birbiri ile kıyaslandı.

Anahtar kelimeler: Modifiye U1 yaklaşımı, Transport Denklemi, Anli-Güngör Saçılması, Difüzyon Katsayısı

1. Introduction

Scientist use different solutions for the nuclear reactor problems since designing of nuclear reactor is quite complex. Neutrons used for the production of energy but neutron behaviors are so complicate in a nuclear power plants. In the system, not only neutrons energy different from each other but also their energy changes with many physical parameters in per collision. For instance reactor criticality generally depend on neutron flux and from this reason scientist must know the flux exactly. To overcome difficult cases related with flux, diffusion approximation is used. This approximation has some advantages for the first estimation of reactor properties such as neutron transport and energy spectrum (Stacey, W. M., (2007); Lamarsh, J. R. & Baratta, A. J. (2001). Neutron diffusion theory provides a simplest and widely used satisfactory mathematical description for the neutron distributions. The diffusion equation relating the current to the gradient of the neutron flux is based on Fick's law, which was originally used to account for chemical diffusion (Lamarsh, J. R. & Baratta, A. J. (2001).

Spherical harmonics method (PN) is mostly used for the calculation of reactor problems such as neutron flux, diffusion length, albedo value, buckling etc. (Yildiz, C. 1998; Güleçyüz, M. C., Şenyiğit ., Ersoy, A., 2018) Case, K.M.,1967). On the other hand, Chebyshev polynomials have been used in the last studies for calculating critical thickness, diffusion length by certain scientists (Anlı F., Yaşa F., Güngör S.& Öztürk H., 2006); Öztürk, H., Anlı, F., & Güngör, S., (2007); Bülbül, A., Ulutas, M., & Anli, F., 2008).

Recently, the workers showed that in their studies UN approximation gives quite coherent results with the widely used PN approximation in literature. Bulbul et al. presented that the second kind of Chebyshev polynomials UN, for isotropic scattering in slab geometry with reflective boundary conditions can be applied to the neutron transport equation (Bülbül, A. Ulutas, M., & Anli, F., 2008). Also modified UN approximation is applied for the solution of criticality problem in slab geometry (Bülbül, A. & Anlı, F. (2009).

In this study, diffusion equation is solved with Chebyshev polynomial expansion which is belong to more general class of one-variable classical polynomials known as ultra-spherical polynomials, denoted by . Each value of λ leads to a different approximation, including the spherical harmonics when λ=1/2[P_N=P_N^(1/2)], Chebyshev polynomials of the second kind when λ=1[U_N=P_N^1]. In the present study, diffusion coefficients are calculated with different scattering function using modified UN method in slab geometry and the results obtained from U1 and P1 approximations are given in the tables for the comparison.

2. Theory

In slab geometry, for the steady-state and time-independent case the neutron transport equation without sources is given as

$$\mu\frac{\partial\psi(x,\mu)}{dx}+\sigma_T\psi(x,\mu)=\frac{\sigma_S}{2}\int_{-1}^{1}\psi(x,\mu')\,d\mu', -a\le x\le a, -1\le\mu\le 1. \quad (1)$$

where $\psi(x,\mu)$ is the angular flux or flux density of neutrons at position *x* traveling in direction μ, σ_T and σ_S are total and scattering differential cross section, respectively. It is aimed to solve Equation (1) with Anli-Güngör scattering function, we use σ_S in terms of AG phase function and it is given as

$$\sigma_S^{AG}(\mu_0) = \frac{\sigma_s}{4\pi(1-2\mu_0 t+t^2)^{1/2}} \;, \qquad -1 \le t \le 1. \quad (2)$$

where σ_S is any non-negative coefficient, the parameter t is in the range of $-1 \le t \le 1$ and $\mu_0 = \mathbf{\Omega}\cdot\mathbf{\Omega'}$ is the cosine of the scattering angel, $\mu_0 = \mu\mu' + \sqrt{1-\mu^2}\sqrt{1-\mu'^2}\cos(\phi-\phi')$.

The conservation of neutron flux equation can be written with the AG phase function given in Eq. (2) as;

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

Using $\int_0^{2\pi}\sigma_S^{AG}(\mu_0)d\phi' = \frac{\sigma_S}{2}\sum_{n=0}^{\infty}t^n P_n(\mu)P_n(\mu')$, the equation can be written

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \nu\psi(x,\mu) = \frac{\nu c}{2}\sum_{n=0}^{\infty}t^n P_n(\mu)\int_{-1}^{1}P_n(\mu')\psi(x,\mu')d\mu' \quad (4)$$

To simplify the derivation of the equations, here a dimensionless space variable such that $\sigma_T x/\nu \to x$ is defined and ν is the eigenvalues. In order to solve Eq.(4), the angular flux is described in terms of modified U_N as

$$\psi(x,\mu) = \frac{2}{\pi}\sum_{n=0}^{N}\Phi_n(x)\,U_n(\mu), -a \le x \le a, -1 \le \mu \le 1 \quad (5)$$

If the neutron angular flux $\psi(x,\mu)$ given in Eq. (5) is inserted into Eq. (4), and the resulting equation is multiplied by $U_n(\mu)$ and integrated over $\mu \in [-1,1]$ using the orthogonality properties and the recurrence relations of the second kind Chebyshev polynomials given below

$$\int_{-1}^{1}U_n(\mu)U_m(\mu)\sqrt{1-\mu^2}d\mu = \begin{cases}\pi/2, n=m\\ 0, n\ne m\end{cases} \quad (6)$$

$$2\mu U_n(\mu) = U_{n+1}(\mu) + U_{n-1}(\mu), -1 \le \mu \le 1 \quad (7)$$

One can obtain the U_N moments of the angular flux for n = 0 and n = 1 respectively

$$\frac{d\Phi_1(x)}{dx} + 2\nu\Phi_0(x) = 2\nu c\sum_{n=0}^{N}\frac{\Phi_{2n}(x)}{2n+1} \quad (8)$$

$$\frac{d\Phi_0(x)}{dx} + \frac{d\Phi_2(x)}{dx} + 2\nu\Phi_1(x) = \frac{2}{3}\nu ct\sum_{n=1}^{N}\frac{\Phi_{2n-1}(x)}{4n^2-1} \quad (9)$$

Eqs. (8) and (9) are U_1 equations of the present method for the neutron transport equation and the condition for n = 1 stated in Eq. (9) is equivalent to diffusion approximation as in spherical harmonics (P_N) method by setting $d\Phi_{N+1}/dx = 0$ (Case, K.M.; Zweifel, P. F.,1967). In the case of U_1 approximation, a familiar equation known as Fick's law is obtained by taking $d\Phi_2/dx = 0$ in Eq. (9),

$$\Phi_1(x) = -\frac{3}{2\nu(3-ct)}\frac{d\Phi_0(x)}{dx} \quad (10)$$

From Eq.(10), diffusion coefficient (D) for modified U_1 approximation can be given,

$$D = \frac{3}{2\nu(3-ct)} \quad (11)$$

By following the same procedure for the P_N approximation, the diffusion coefficient which depends on c and t parameters can be obtained for the P_1 method as,

$$D = \frac{1}{v(3-ct)} \tag{12}$$

In Fick's Law current is given as a function of flux and the equation depends on diffusion coefficient as

$$J = -D\nabla\Phi \tag{13}$$

In the present study, Eq. (10) is the current term and one could obtain *D* for modified *U₁* method simply according to Eq.(13). In addition, diffusion length depends on diffusion coefficient and macroscopic absorption cross section as $L = (\frac{D}{\sum_a})^{1/2}$ and total macroscopic cross section is given as $\sum_t = \sum_a + \sum_s$. In Eqs. (11-12), the parameter ν related to the total macroscopic cross section $\sum_t$ and $v = \sum_t$ is given. One obtain diffusion coefficient for modified U_1 as $D = \frac{3}{2\sum_t(3-ct)}$ and using total macroscopic cross section in this term, *D* values can be obtained for certain moderators.

3.Results

In this study, diffusion coefficients are calculated for different collision parameters and scattering parameters. Modified U_1 approximation is applied to diffusion problem using AG phase function in slab geometry then diffusion coefficients are given Table 1 and Table 2 for the comparison with P_1 approximation. It can be said from the present method, modified U_1 approximation gives acceptable results with P_1 approximation.

Table 1. Diffusion coefficients *D* (cm) values obtained from P_1 and U_1 approximations for *c* = 0.9999, 0.9888 and 0.9600 and different values of *t* with AG phase function

t	*c* = 0.9999		*c* = 0.9888		*c* = 0.9600	
	U_1	P_1	U_1	P_1	U_1	P_1
0.00	0.50000	0.33333	0.50000	0.33333	0.50000	0.33333
0.25	0.54545	0.36363	0.54490	0.36326	0.54348	0.36232
0.50	0.59999	0.39999	0.59866	0.39911	0.59524	0.39683
0.70	0.65215	0.43477	0.64996	0.43331	0.64433	0.42955
0.85	0.69765	0.46510	0.69460	0.46307	0.68681	0.45788
1.00	0.74996	0.49998	0.74582	0.49722	0.73529	0.49020

Table 2. Diffusion coefficents *D* (cm) values obtained from P_1 and U_1 approximations for *c* = 0.9000, 0.8999 and 0.8500 and different values of *t* with AG phase function

t	*c* = 0.9000		*c* = 0.8999		*c* = 0.8500	
	U_1	P_1	U_1	P_1	U_1	P_1
0.00	0.50000	0.33333	0.50000	0.33333	0.50000	0.33333

0.25	0.54054	0.36036	0.54054	0.36036	0.53812	0.35874
0.50	0.58824	0.39216	0.58822	0.39215	0.58252	0.38834
0.70	0.63291	0.42194	0.63289	0.42193	0.62370	0.41580
0.85	0.67114	0.44743	0.67112	0.44741	0.65862	0.43908
1.00	0.71429	0.47619	0.71425	0.47617	0.69767	0.46512

On the other hand, if one analysis isotropic scattering for slab geometry, the scattering parameter must be get $t = 0$ in equation.

Calculation of diffusion coefficient is necessary for the estimation of reactor size and components. In a reactor, diffusion approximation is rough but it is used generally for the first calculation. Using total macroscopic cross section value of moderators, D values can be obtained.

4.Conclusion

In literature, diffusion approximation is known the first-order approximation and it is used for the first calculations of a reactor. Especially, it is used when c is near to unity but this approximation is not usable for a strongly absorbing medium. The purpose of this study is to show the solution of diffusion equation with modified U_1 method using a new scattering function. As with the P_1 approximation, it makes sense to write, the diffusion equation based on flux and obtain new sets of equations. However, the method used and the scattering function are not claimed to be the best.

Theoretical solutions are necessary for the best designing of a reactor. Since, diffusion approximation is related to calculation of neutron flux, it is used conventionally on determination of reactor components such as material composition and reactor size. The results of theoretical approximations give first estimation to scientist about the some problems such as environment, economy, safety energy and technical needing.

Consequently, first order approximation was investigated for the calculation of diffusion coefficient and it was seen that the results of modified U_N approximation were comparable with P_N results. Briefly, it can be said that new scattering function and U_N approximation may be applied to any problem in engineering, physics, optic, etc. It is planned to apply the improved form of polynomial technique in the next study.

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