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Variable Separation and Boubaker Polynomial Expansion Scheme for Solving the Neutron Transport Equation

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Abstract: Problem statement: In this study, we present general analytical solutions to the Neutron Boltzmann Transport Equation NBTE using a polynomial expansion scheme. **Approach:** Some simple assumptions have been introduced in the main system thanks to the Boubaker Polynomial Expansion Scheme (BPES) in order to make the general analytical procedure simple and adaptable for solving similar real life problems. **Results:** Finding particular solution to the Neutron equation by making use of boundary conditions and initial conditions may be too much for the present study and reduce the generality of the solutions. **Conclusion:** The proposed analytical solution of the neutron transport equation has been positively compared to some recently publish results. I should present a relevant supply to studies on reactor modeling.

Key words: Neutron transport equation, distribution function, Boubaker Polynomial Expansion Scheme (BPES), source function, neutron angular flux, analytical solutions, seems appropriate, describing neutron, boltzmann equation

INTRODUCTION

The deterministic neutron transport equation (or Boltzmann neutron transport equation) describes the expected or probable neutron angular density with respect to position, direction, energy and time. Is solutions generally provide average values of the neutron angular density which takes into account random effects from neutron interactions and sources. Since neutrons are neutral particles which possess mass, they can penetrate deep into matter in a nondestructive way despite having characteristics strong forces, a quantum mechanical description seems appropriate, leading to an involved system of Schrödinger equations describing neutron motion between and within nuclei (Kulikowska, 2000; Lewis and Miller, 1984; Bell and Glasstone, 1970; Stammler and Abbate, 1983; Singh, *et al*., 2010;Nourazar *et al.* , 2011).

From a theoretical point of view, a neutron is a neutral point particle, experiencing deflection from or capture by a nucleus at the center of an atom. If the conditions are just right, the captured neutron causes a fissile nucleus to fission, producing more neutrons. A stochastic partial differential equation is hence derived from these events of neutron transport in a general three-dimensional absorbing and anisotropic-scattering medium where the neutron angular density depends on position, direction, energy and time (Lewis and Miller, 1984). Sometimes, the nucleus that remains as fission product coincides with one of the stable nuclei. The product nucleus is then different from other nuclei, the reason being that the product nucleus is not stable. It disintegrates further, with a mean life characteristic of the nucleus, by emission of an electric charge, until it finally reaches a stable state.

In the present investigation, the medium is assumed to be constant with respect to material composition, i.e., zero power noise. Special random effects, for example, from randomly varying boundary conditions or from a medium that is randomly varying are not considered in the present investigation although generalizations to approximate such conditions may be possible.

MATERIALS AND METHODS

The neutron transport equation models the transport of neutral particles in a scattering, fission and absorption set of events with no self-interactions (Lewis and Miller, 1984; Chandrasekhar, 1960; Davison, 1957).

In a neutron scattering event (Fig. 1), the quantity to be determined is called the partial differential cross section related to $\Delta\Omega$. This function depends on the energy and momentum transferred from the neutron to the sample. In the most general case the partial differential cross section is a function of four variables since the momentum transfer is a vector quantity with

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three components. In elastic scattering, the neutron does not transfer any energy to the sample. The elastic differential cross section is consequently a function of momentum transfer only. From the number of neutrons counted in a detector, the mean values for variables θ and ϕ can be defined (Fig. 1). θ is the angle through which the neutron has been scattered, i.e. the angle between the incident and the scattered beam.

The paths of the neutrons which are scattered through θ form a cone so a second (azimuthal) angle, ϕ, is also needed to define the detector position. Several analytical and numerical approaches have been used in order to solve the neutron transport equation. Jaffel and Vidal-Madjar (1989); Case and Hazeltine (1970) and Davies (2002) performed dicretizing protocols based on Fourier transform, while Cardona and Vilhena (1994); Kim and Ishimaru (1999); Kim and Moscoso (2002); Boyd (2001); Bernardi and Maday (1992) and Kadem (2008) used polynomial expansion schemes..

In the actual investigation, the first assumption is that all particles including nuclei are in motion with like particle collisions allowed, as stated by Kulikowska (2000); Mokhtar-Kharroubbi (1997) and Kadem (2006). The govening equation are Eq. 1:

$$\begin{aligned}&\left\{\frac{1}{v}\frac{\partial}{\partial t}+\Omega.\nabla+\Sigma(r,E,t)\right\}\psi(r,\Omega,E,t)=\\&\int_0^\infty dE'\int_{4\pi}d\Omega'\Sigma_s(r,\Omega'.\Omega,E'\to E)\psi(r,\Omega',E',t)\\&+\frac{\chi(E)}{4\pi}\int_0^\infty dE'\int_{4\pi}d\Omega' V_E(E')\Sigma_f(r,E',t)\psi\\&(r,\Omega',E',t)=Q(r,\Omega,E,t)\end{aligned}\tag{1}$$

With:

V	=	The neutron speed
Σ,Σ_f	=	Macroscopic cross-sections
Σ_s	=	Scattering cross-section
χ (E)	=	The distribution function
ψ	=	The neutron angular flux
E,E'	=	Energies
Ω, Ω'	=	Neutron directions
Q(r,Ω,E,t)	=	The source function (Kulikowska, 2000)

Which give, using variable separation Eq. 2:

$$\begin{aligned}&\frac{\psi_2}{v}\frac{\partial\psi_1}{\partial t}+\Omega\psi_2.\nabla\psi_1+\Sigma_1\Sigma_2\Sigma_3\psi_1\psi_2=\psi_1\Sigma_{s1}(r)\\&\int_0^\infty dE'\int_{4\pi}d\Omega'\Sigma_{s2}(\Omega'.\Omega,E'\to E)\psi'_2+\frac{\chi(E)}{4\pi}.\\&\psi_1\psi'_2\int_0^\infty dE'\int_{4\pi}d\Omega' V_E(E')\Sigma_{f1}\Sigma_{f2}\Sigma_{f3}+Q(r,\Omega,E,t)\end{aligned}\tag{2}$$

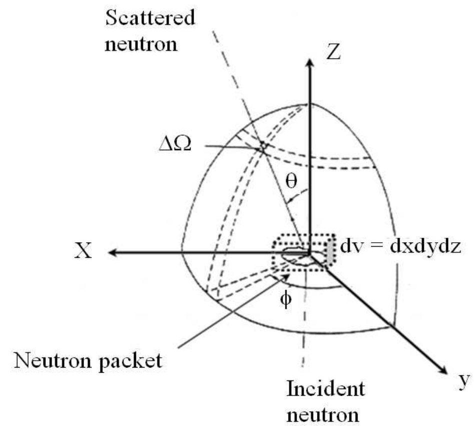

Fig. 1: Neutron scattering event geometrical model

which gives Eq. 3:

$$\begin{aligned}&\frac{\psi_2}{v}\frac{\partial\psi_1}{\partial t}+\Omega\psi_2\frac{\partial\psi_1}{\partial r}+\\&\left\{\begin{aligned}&\Sigma_1\Sigma_2\Sigma_3\psi_2-\psi'_2\Sigma_{s1}(r)\\&\int_0^\infty dE'\int_{4\pi}d\Omega'\Sigma_{s2}-\frac{\chi(E)}{4\pi}.\psi'_2\Sigma_{f1}(r)\Sigma_{f3}\\&(t)\int_0^\infty V_E(E')\Sigma_{f2}(E')dE'\int_{4\pi}d\Omega'\end{aligned}\right\}\psi_1=Q\end{aligned}\tag{3}$$

where, V_E represents the average number of neutrons per fission.

By setting Eq. 4:

$$\begin{aligned}&\psi_1(r,t)=R(r)G(t)\\&A(r,t)=A_1(r)+A_2(t)\\&Q_1(r,t)=\psi_1Q_0\\&Q_0=Q_0(r)+G_0(t)\end{aligned}\tag{4}$$

One obtains:

$$\begin{aligned}&\frac{\psi_2}{Q_2v}R\frac{dG}{dt}+\frac{\Omega\psi_2}{Q_2}G\frac{dR}{dr}+\left\{\frac{A_1(r)+A_2(t)}{Q_2}\right\}\\&RG=RG(R_0+G_0)\frac{\psi_2}{Q_2v}\frac{1}{G}\frac{dG}{dt}+\frac{\Omega\psi_2}{Q_2}\frac{1}{R}\frac{dR}{dr}\\&+\frac{A_1(r)}{Q_2}+\frac{A_2(t)}{Q_2}=(R_0+G_0)\frac{\psi_2}{Q_2v}\frac{1}{G}\frac{dG}{dt}+\\&z\frac{\Omega\psi_2}{Q_2}\frac{1}{R}\frac{dR}{dr}+\frac{A_1(r)}{Q_2}+\frac{A_2(t)}{Q_2}=(R_0+G_0)\\&\frac{\psi_2}{Q_2v}\frac{1}{G}\frac{dG}{dt}+\frac{A_2(t)}{Q_2}-G_0(t)=-\\&\frac{\Omega\psi_2}{Q_2}\frac{1}{R}\frac{dR}{dr}-\frac{A_1(r)}{Q_2}+R_0(r)\end{aligned}\tag{5}$$

Since both sides of Eq. 5 are independent of one another, they must be equal to a constant ε^2; leading to the following equations Eq. 6 and 7:

$$\frac{dG}{dt} = \frac{Q_2 v}{\psi_2}\left\{G_0(t) - \frac{A_2(t)}{Q_2} + \varepsilon^2\right\}G(t) \tag{6}$$

$$\frac{dR}{dr} = \frac{Q_2}{\Omega\psi_2}\left\{R_0(r) + \varepsilon^2 - \frac{A_1(r)}{Q_2}\right\}R(r) \tag{7}$$

which have as solutions Eq. 8 and 9:

$$G(t) = P_0 e^{\frac{Q_2 v}{\psi_2}\int\left\{G_0(t) - \frac{A_2(t)}{Q_2} + \varepsilon^2\right\}dt} \tag{8}$$

$$R(r) = P_1 e^{\frac{Q_2}{\Omega\psi_2}\int\left\{R_0(r) + \varepsilon^2 - \frac{A_1(r)}{Q_2}\right\}dr} \tag{9}$$

where, P_0 and P_1 are constants.

The expression for the flux is hence given as Eq. 10:

$$\begin{cases} \psi(r,\Omega,E,t) = P_0 P_1 \psi_2(\Omega,E) e^{\frac{Q_2}{\psi_2}(\mu_1+\mu_2)} \\ \mu_1 = v\int\left\{G_0(t) - \frac{A_2(t)}{Q_2} + \varepsilon^2\right\}dt \\ \mu_2 = \frac{1}{\Omega}\int\left\{R_0(r) + \varepsilon^2 - \frac{A_1(r)}{Q_2}\right\}dr \end{cases} \tag{10}$$

RESULTS

Different expressions to Q_2, G_0, A_2, A_1 and R_o allow obtaining different expressions of the macroscopic cross section which is generally expressed as Eq. 11:

$$\Sigma_{ij}(r,E,t) = N_j(r,t)\sigma_{ij}(E) \tag{11}$$

For a given nuclide j and reaction type i, where N_j (r, t) is the nuclear atomic density and σ_{ij} (E) is the microscopic cross section, then, if we assume that nuclear atomic density is independent of time Eq. 12 and 13:

$$\Sigma_{ij} = N_j(r)\sigma_{ij}(E) \tag{12}$$

Then:

$$\begin{cases} \Sigma_3(t) = 1 \\ \Sigma(r,E) = \Sigma_1(r)\Sigma_2(E) \end{cases} \tag{13}$$

And the expression for the distribution function $\chi(E)$ becomes (Kulikowska, 2000; Kadem, 2006; Mokhtar-Kharroubbi, 1997) Eq. 14:

$$\begin{gathered} \frac{\chi(E)}{4\pi}\psi_2'\Sigma_{f1}(r)\int_0^\infty V_E(E')\Sigma_{f2}(E')dE'\int_{4\pi} d\Omega' = \Sigma_1(r)\Sigma_2(E) \\ \psi_2 - A(r) - \psi_2'\Sigma_{s1}(r)\int_0^\infty \Sigma_{sb}(E' \to E)dE'\int_{4\pi}\Sigma_{sa}(\Omega'.\Omega)d\Omega' \\ \chi(E) = \frac{4\pi\Sigma_1(r)\Sigma_2(E)\psi_2 - 4\pi A(r) - 4\pi\psi_2'\Sigma_{s1}(r)\int_0^\infty \Sigma_{sb}(E' \to E)dE'\int_{4\pi}\Sigma_{sa}(\Omega'.\Omega)d\Omega'}{\psi_2'\Sigma_{f1}(r)\int_0^\infty V_E(E')\Sigma_{f2}(E')dE'\int_{4\pi} d\Omega'} \end{gathered} \tag{14}$$

DISCUSSION

Criticality and analytical solutions can be discussed by considering the special case of the neutron transport equation without delayed neutrons, which is traduced by the equation:

$$\begin{aligned} &\left\{\frac{1}{v}\frac{\partial}{\partial t} + \Omega\nabla + \sigma(\vec{r},E)\right\}\psi(\vec{r},\Omega,E,t) = Q_{ext}(\vec{r},\Omega,E,t) \\ &+\int dE'\int d\Omega'\sigma_s(\vec{r},\Omega'.\Omega,E' \to E)\psi(\vec{r},\Omega,E',t) \\ &+\chi(E)\int dE'\int d\Omega' V_E\sigma_f(\vec{r},E')\psi(\vec{r},\Omega',E',t) \end{aligned} \tag{15}$$

With:

Q_{ext} = The external sources of neutrons
σ = The microscopic cross-section
v = The neutron speed
V_E = Average number of neutrons per fission

This equation assumes that all neutrons are emitted instantaneously at the time of fission although small fraction of neutrons is emitted later due to certain fission products.

If we look for an asymptotic solutions to Eq. 15, satisfying the source free boundary conditions (Q_{ext} = 0), it gives:

$$\begin{aligned} B(\vec{r}) = &\frac{\sigma_{s1}(\vec{r})}{\psi_{a3}(E)}\int\sigma_{s2}(E' \to E)\,\psi_{a3}'(E')dE' \\ &\int\sigma_{s3}(\Omega'.\Omega)\psi_{a2}d\Omega' - \frac{\alpha}{v} - \sigma_1(\vec{r})\sigma_2(E) \\ &+\frac{\chi(E)V_E}{\psi_{a2}(\Omega)\psi_{a3}(E)}\int\sigma_{f2}(E')\,\psi_{a3}'(E')dE' \\ &\int\sigma_{f1}(\vec{r})\,\psi_{a2}'(\Omega')d\Omega' \end{aligned} \tag{16}$$

And:

$$\Omega\frac{d\psi_{a1}}{dr} = B(\vec{r})\psi_{a1} \tag{17}$$

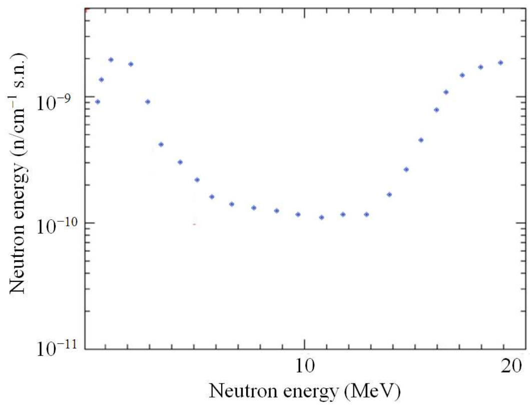

Fig. 2: Energy-dependent neutron flux profile

If we suppose that the integral $\int_0^\infty \frac{B(\vec r)}{\Omega} d\vec r$ is convergent and taking into account the characteristics of a given nuclear reactor with spherical symmetry ($B(\vec r) = \|B(\vec r)\|\frac{\vec r}{\|\vec r\|} = \|B(\vec r)\|\vec u_r$ within radial range [0, R]:

$$\begin{cases} B(\vec r)\big|_{\vec r=\vec 0} = k_1 \\ \dfrac{d\|B(\vec r)\|}{dr}\Big|_{\vec r=\vec 0} = 0 \\ B(\vec r)\big|_{\vec r=R\vec u_r} = 0 \\ \dfrac{d\|B(\vec r)\|}{dr}\Big|_{\vec r=R\vec u_r} = k_2 \end{cases} \tag{18}$$

where, k_1 k_2 are core reactor characteristic constants.

For solving Eq. 16-17, the Boubaker Polynomials Expansion Scheme BPES is proposed. This scheme is applied through setting the expression:

$$\|B(\vec r)\| = \frac{1}{2N_0}\sum_{k=1}^{N_0}\lambda_k \times B_{4k}\left(\frac{r}{R}\mu_k\right) \tag{19}$$

where, B_{4k} are the 4k-order Boubaker polynomials, r is the radius ($r \in [0, R)$),μ_k are B_{4k} minimal positive roots, N_0 is a prefixed integer and $\lambda_k\big|_{k=1..N_0}$ are unknown pondering real coefficients.

At this stage, the main advantage of this step lies in Eq. 19 which ensures verifying the four boundary conditions in Eq. 18, at the earliest stage of resolution protocol. In fact, due to the properties of the Boubaker polynomials (Ghanouchi *et al*., 2007; Awojoyogbe and Boubaker, 2009; Labiadh and Boubaker, 2007; Slama *et al*., 2009; Hossein *et al*., 2009; Fridjine and Amlouk, 2009; Belhadj *et al*., 2009a; 2009b, Barry and Hennessy, 2010; Agida and Kumar, 2010;Yildirim *et al*., 2010; Kumar, 2010; Milgram, 2011) and since $\mu_k\big|_{k=1..N_0}$ are roots of $B_{4k}\big|_{k=1..N_0}$, Eq. 15 is reduced to Eq. 20:

$$\begin{cases} \sum_{k=1}^{N_0}\lambda_k \times B_{4k}\left(\frac{r}{R}\mu_k\right)\Big|_{\vec r=\vec 0} = \sum_{k=1}^{N_0}\lambda_k \times (-2) = 2k_1N_0 \\ \sum_{k=1}^{N_0}\lambda_k \times \dfrac{dB_{4k}\left(\frac{r}{R}\mu_k\right)}{dr}\Bigg|_{\vec r=\vec 0} = \sum_{k=1}^{N_0}\lambda_k \times 0 = 0 \\ \sum_{k=1}^{N_0}\lambda_k \times B_{4k}\left(\frac{r}{R}\mu_k\right)\Big|_{\vec r=R\vec u_r} = \sum_{k=1}^{N_0}\lambda_k \times B_{4k}(\mu_k)\big| = 0 \\ \sum_{k=1}^{N_0}\lambda_k \times \dfrac{dB_{4k}\left(\frac{r}{R}\mu_k\right)}{dr}\Bigg|_{\vec r=R\vec u_r} = \sum_{k=1}^{N_0}\lambda_k \times \\ \dfrac{dB_{4k}(\mu_k)}{dr} = \sum_{k=1}^{N_0}\lambda_k \times H_k = 2k_2N_0 \\ \text{with}: H_k = \dfrac{dB_{4k}\left(\frac{r}{R}\mu_k\right)}{dr}\Bigg|_{\vec r=R\vec u_r} = \\ \left(\dfrac{4\mu_k[2-\mu_k^2]\times\sum_{j=1}^{k}B_{4j}^2(\mu_k)}{B_{4(k+1)}(\mu_k)} + 4\mu_k^3\right) \end{cases} \tag{20}$$

The solution is then assigned to the set of pondering real coefficients $\tilde\lambda_k\big|_{k=1..N_0}$ which minimizes the Minimum Square functional Ψ_{N0}:

$$\Psi_{N_0} = \left(\sum_{k=1}^{N_0}\tilde\lambda_k \times (-2) - 2k_1N_0\right)^2 + \left(\sum_{k=1}^{N_0}\tilde\lambda_k \times H_k = 2k_2N_0\right)^2 \tag{21}$$

Which gives the following solution to Eq. 21:

$$\psi_a(\vec r) = P_3 e^{\int \frac{\frac{1}{2N_0}\sum_{k=1}^{N_0}\tilde\lambda_k \times B_{4k}\left(\frac{r}{R}\mu_k\right)}{\Omega} d\vec r} \tag{22}$$

With P_3 constant.

From Eq. 22 and our earlier assumptions, we write Eq. 23:

$$\psi_a(\vec r, \Omega, E) = P_3\psi_{a2}(\Omega)\psi_{a3}(E)\int \frac{\frac{1}{2N_0}\sum_{k=1}^{N_0}\tilde\lambda_k \times B_{4k}\left(\frac{r}{R}\mu_k\right)}{\Omega} d\vec r \tag{23}$$

$$\psi(\vec{r},\Omega,E,t) = P_3\psi_{a2}(\Omega)\psi_{a3}(E)e^{\alpha t+\int \frac{\frac{1}{2N_0}\sum_{k=1}^{N_0}\tilde{\lambda}_k \times B_{4k}(\frac{r}{R}\mu_k)}{\Omega}d\vec{r}} \quad (24)$$

Figure 2 presents the profile of the energy-dependent neutron flux as per Eq. 24. The obtained patterns are in good agreement with the results recorded by Lent *et al*. (2004); Zeyad *et al*. (2007) and Zhao *et al*. (2006).

CONCLUSION

An analytical solution of the neutron transport equation applying the Boubaker Polynomial Expansion Scheme BPES has been presented. The solution plots and main features have shown a good agreement with some recently published results and should present a relevant supply to studies on reactor modeling. Effects of power noise, special random effects and variable boundary conditions are subjects of future studies.

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