Characteristics of neutron diffusion coefficient as a function of energy group in the one-dimensional multi-group diffusion equation of finite slab reactor core

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Abstract. One of the most straightforward approaches that widely used to solve the neutron transport equation is the diffusion equation approach. The diffusion equation describes the individual behavior of the average neutron trajectory when interacting with matter. Usually, the neutron diffusion equation is obtained under the assumption that scattering is isotropic in the laboratory system of coordinates, and neutrons have the same energy and region is homogeneous; this called a one-speed diffusion equation. It leads to the diffusion coefficient to be independent of the spatial position; the volume of the reactor is constant, and the number density of the fuel atoms is also relatively constant. In this study, multi-group neutron diffusion characteristics were introduced in two ways. First, they vary with energy in the finite slab reactor core using a one-dimensional multi-group diffusion equation with the Gauss-Seidel iteration method. Second, using Fick's law directly. The study used macroscopic cross-sections in the U-PuN fuel cell level as initial input for 70 energy groups. The data library used is JFS-3-J33 for 70 energy groups, which is the library data of SLAROM computer codes from JAEA Japan. The first way indicates the diffusion coefficient characteristics of U-235 and Pu-239 fuel isotopes firmly have the same pattern in each energy group. They have fluctuations throughout the fast, intermediate, and thermal energy group regions because both isotopes are fertile material. On the other hand, the diffusion coefficient of U-238 fuels isotope tends to be stable in each energy group. This event occurs because the isotope of U-238 is natural uranium, which is included as a fertile material. The second way shows the diffusion coefficients characteristics of the nuclear fuel isotopes firmly have the same pattern in each energy group, especially in the fast and thermal energy group region. They have fluctuations only throughout the intermediate energy group regions because, in this area, there is a resonant region.

1. Introduction
In the operation of nuclear reactors, it is noteworthy to estimate how the neutrons will be distributed throughout the reactor core. The neutron transport equation explains the occurrence of neutron population events that illustrates the balance between all nuclear processes. Unfortunately, in general,
determining the neutron distribution is a complicated problem. Neutrons in reactors core move in complicated paths as a result of repeated nuclear collisions [1]. Estimated values of neutron distribution can be found by solving diffusion equations such as equations used to describe diffusion phenomena in engineering, such as molecular transport. One of the simplest approaches that have been widely used in research and practice to solve the neutron transport equation is the diffusion equation approach [2,3]. The diffusion equation describes the individual behavior of the average neutron trajectory when interacting with matter. This interaction will produce how fast one material can diffuse through another material. In this case, the interaction of neutrons with nuclear fuel material is studied to determine how much the neutron experiences to leakage, fission, absorption, or scattering. The neutron diffusion equation is a mathematical model suitable for making critical and balance calculations of neutrons in nuclear reactors [3].

Usually, the neutron diffusion equation is obtained under the assumption that scattering is isotropic in the laboratory system of coordinates, neutrons have the same energy, and the region is homogeneous; this called a one-speed diffusion equation [4]. This assumption leads to the diffusion coefficient to be independent of the position in space; the volume of the reactor is constant, and the number density of the fuel atoms is also relatively constant. Since the atom density and microscopic cross-section are not varying with energy, then the macroscopic cross-section must be continuous.

The neutrons have a broad energy spectrum, ranging from a fraction of an eV to a few MeV, the cross-sections vary over decades in this range, so it can hardly expect the one-group approximation to be very accurate. Based on these reasons, this study uses a multi-group approach to resolve the diffusion coefficient as a function of energy. Ideally, the few-group constants, including the diffusion coefficient, is resulted from the calculation of assembly [5]. Once the assembly calculation is done, the cross-sections are spatially homogenized, and a critical spectrum calculation is performed to take into account the neutron leakages of the lattice. The diffusion coefficient is also generated through the critical spectrum calculation.

In the preliminary study [6], the calculation of neutron flux distribution has been done by assuming the neutron diffusion coefficient is independent of the energy group. The current study presents the neutron diffusion coefficient varies with energy in the finite slab reactor core using a one-dimensional multi-group diffusion equation with the Gauss-Seidel iteration method. The finite slab reactor core means that neutron leakage could be considered for the moment as a destructive process [7]. The macroscopic cross-sections data used in this study is executed from the result of the computer program development [8], which is the U-PuN fuel cell level as initial input for 70 energy groups. The data library used is JFS-3-J33 70 energy groups, which is the library data of SLAROM computer codes from JAEA Japan [9]. The solution of the one-dimensional multi-group diffusion equation, in this study, uses the Gauss-Seidel iteration method. However, the residual power series method [10] and the Jacobi iteration method [6] can also be used. As a comparison, the results of the diffusion coefficient calculation are also presented by applying Fick's law [4] by inserting the multi-group transport cross-section directly [5].

2. Theoretical background

Based on the concept of neutron equilibrium in the reactor core, the general form of multi-group neutron diffusion equation which describes the leakage, absorption, scattering, fission production, and the external source follows [4]

$$\frac{1}{v_g} \frac{\partial \phi_{g}}{\partial t} = \nabla \cdot D_g \nabla \phi_{g} - \Sigma_{ag} \phi_{g} + S_{g} - \Sigma_{bg} \phi_{g} + \sum_{g'=1}^{G} \Sigma_{bg'g} \phi_{g'}$$  \hspace{1cm} (1)

where $g$ is an index of energy group, $v_g$ is the neutron speed, neutron flux $\phi_{g}$, diffusion coefficient $D_g$, $\Sigma_{ag}$ and $\Sigma_{bg}$ is the macroscopic cross-section of absorption and scattering in the point $r$ and energy group $g$, and $S_g$ is the neutron source. Equation (1) Equation (1) can be solved using several approaches:
The boundary conditions at the end of the reactor core have zero neutron flux, as well as the neutron source (void boundary condition).

- Only macroscopic scattering cross-section in the fuel material has been considered.
- No neutrons can be absorbed in the materials.
- Neutron is at the steady-state condition.

Based on the previous assumptions, Equation (1) can be simplified into the one-dimensional multi-group diffusion equation as follows

$$-D_g \nabla^2 \phi_g (x) + \Sigma_{sg} \phi_g (x) = S_g (x)$$  \hspace{1cm} (2)

Substitution Laplacian operator and by using the discretization central finite difference model into Equation (1) then Equation (2) becomes to

$$\frac{\phi_{g(i+1)x} - 2\phi_g + \phi_{g(i-1)x}}{(\Delta x)^2} - \frac{\Sigma_{sg} \phi_g}{D_g} = -\frac{S_g}{D_g}$$ \hspace{1cm} (3)

By using the Gauss-Seidel iteration method, neutron flux distribution in the Equation (3) becomes to

$$\phi_{g(n+1)x} = \frac{S_{ix} + \phi_{g(i+1)x} + \phi_{g(i-1)x}}{D_g}$$ \hspace{1cm} (4)

Finally, the multi-group neutron diffusion coefficient is expressed in the form

$$D_{ig} = \frac{(\Sigma_{sig} \phi_{ig} - S_{ig}) \Delta x^2}{(\phi_{g(i+1)x} - 2\phi_{g(i)x} - \phi_{g(i-1)x})}$$ \hspace{1cm} (5)

where $\Delta x$ is a spatial mesh of core width, and $i$ is an index of mesh instead of the $x$-axis. Multi-group neutron diffusion coefficient also can be calculated using Fick's law directly as follows [5]

$$D_g = \frac{1}{3 \Sigma_{sig}}$$ \hspace{1cm} (6)

$\Sigma_{sig}$ here is $\Sigma_{sig}$ namely, neutron transport macroscopic cross-sections, but based on the above assumptions, then $\Sigma_{sig}$ is replaced by $\Sigma_{sig}$ because only the neutron scattering process involves in this study.

3. Design and computational method

The geometry of the finite slab reactor core design using void boundary conditions with spatial mesh $\Delta x$ is shown in Figure 1. The nuclear fuel used in this study is U-PuN with a data library using JFS-3-J33 of SLAROM computer codes for 70 energy groups [9]. The reactor core is composed of several homogeneous nuclear fuel cells. The consequence is the macroscopic cross-section inside the reactor core is homogeneous too and independent on spatial mesh. In this study, the multi-group diffusion equation for calculating the neutron diffusion coefficient considers in the $x$-direction only. Given only one dimension, the height of the reactor core can be ignored.

![Figure 1. The finite slab reactor core model [6].](image-url)
The boundary condition that satisfies Figure 1 for neutron flux and neutron source at the point $x = 0$ and $x = L$ are

$$
\phi_x (0) = \phi_x (L) = 0 \quad \text{and} \quad S_x (0) = S_x (L) = 0
$$

(7)

The computation procedures to calculate the neutron diffusion coefficient follows:

1. Enter the initial neutron flux and neutron source input for all energy groups.
2. Determine the boundary conditions and mesh spatial variable based on Equation (7) in the finite slab reactor core with length 20 cm.
3. Import the previous data [8] of the multi-group macroscopic scattering cross-section of U-PuN fuel cells.
4. Firstly, calculate the neutron flux in each region and energy group using Equation (4) and save it as a preliminary calculation of multi-group neutron diffusion coefficient using Equation (5).
5. Calculate the multi-group diffusion coefficient directly using Equation (6).

4. Results and discussion

The neutron flux distribution in the reactor core is determined by the atomic density of each nuclear fuel isotopes, which is closely related to the macroscopic fission, absorption, and scattering cross-section. Because neutrons are neutral, they can travel a great distance when they become interaction with the material; as a result, neutrons being attenuation. If the isotope formed in the neutron flux is unstable, then the isotope will decay when the isotope is formed.

![Figure 2](image-url)

**Figure 2.** Multi-group neutron diffusion coefficient of the nuclear fuel isotopes.

Figure 2 shows the characteristics of the multi-group neutron diffusion coefficient when neutrons interact with U-235, U-238, and Pu-239 isotopes in the finite slab reactor core with length 20 cm. The diffusion coefficients of U-235 and Pu-239 firmly have the same pattern in each energy group. They have fluctuations throughout the fast, intermediate, and thermal energy group regions. The fast energy region is represented by group 1 to group 19, the slowing down energy range is represented by the group 20 to the group 37, and the thermal energy range is represented by group 38 to group 70 [11]. Besides, the magnitude of the diffusion coefficient value of U-235 is slightly higher than that of Pu-239. The phenomenon is perceptible because both of isotopes are fertile material, i.e., material that is easy to fission and has a higher probability of fission compared to the neutron capture reaction, even though it is pulverized with a low-energy neutron. Heavy nuclides will split into two parts if they absorb neutrons, and at the same time, it will emit 2-3 neutrons.
Different patterns are experienced by the isotope U-238, where along with the energy group, the diffusion coefficient tends to be constant. This event occurs because the isotope of U-238 is natural uranium, which is included as a fertile material, i.e., material that has the potential to be converted into fissile material with a neutron capture reaction. Natural uranium is the most available in nature, which is around 99.2% [1-4]. In addition, the scattering cross-section does not vary significantly along with the energy group. The neutron flux will increase very slowly due to the burn-up of the fuel and resulting decrease in atom density and macroscopic cross-section.

5. Conclusions

There are two ways to calculate the neutron diffusion coefficient characteristics when neutrons interact with U-PuN in the finite slab reactor core. First, the multi-group neutron diffusion coefficient as a function of 70 energy groups is calculated using the Gauss-Seidel iteration method with length 20 cm. It indicates the diffusion coefficients of U-235 and Pu-239 fuel isotopes firmly have the same pattern in each energy group. They have fluctuations throughout the fast, intermediate, and thermal energy group regions because both isotopes are fertile material. On the other hand, the diffusion coefficient of U-238 fuels isotope tends to be stable in each energy group. This event occurs because the isotope of U-238 is natural uranium, which is included as a fertile material.

Another way to calculate the diffusion coefficient is to apply Fick's law directly, assuming the transport event is dominated by neutron scattering so that the macroscopic transport cross-section is replaced with a macroscopic scattering cross-section. The diffusion coefficients of the nuclear fuel isotopes closely have the same pattern in each energy group, especially in the fast and thermal energy group.

Figure 3. Multi-group neutron diffusion coefficient of the nuclear fuel isotopes using Fick's law.

Figure 3 shows that the characteristics of the multi-group neutron diffusion coefficient of the nuclear fuel isotopes using Fick's law directly. In this calculation, macroscopic scattering cross-section is taken directly from the count of the nuclear fuel cells [8] using Equation (6), so the width of the reactor core is ignored. Therefore, the diffusion coefficient value is higher than the calculation using the Gauss-Seidel iteration on the Equation (5). The diffusion coefficients of the nuclear fuel isotopes firmly have the same pattern in each energy group, especially in the fast and thermal energy group region. They have fluctuations only throughout the intermediate energy group regions because, in this area, there is a resonant region. In the resonant region, the absorption cross-section increases by orders of magnitude over a very narrow energy range [1]. Figures 1 and 2 also show that U-235 nuclides are more dominant than U-238 and Pu-239 nuclides. This means that the interaction of neutrons with the fuel constituents causes the neutrons to travel longer for fissile nuclides than for fertile nuclides.
They have fluctuations only throughout the intermediate energy group regions because, in this area, there is a resonant region. This interaction will produce how fast one material can diffuse through another material.

Acknowledgments
The author thanks to the Directorate of Research and Community Service, Directorate General of Strengthening Research and Development, Ministry of Research, Technology, and Higher Education, with Research Contract No: 63/SP2H/AMD/LT/DRPM/2020 for supporting fund in the Fundamental Research scheme.

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