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Application of The Computational Semi-Empirical Method in Calculating The Fission Yield with Reference to The JENDL Data

Rizal Kurniadi[1]
[1]*Nuclear Physics and Bio Physics Research Group, Institut Teknologi Bandung, INDONESIA*

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Abstract

Fission Yield calculation techniques can be completed in various ways. In this work, other calculation techniques will be described. Namely, a semi-empirical technique that utilizes random numbers. This semi-empirical method can produce fitting parameters to obtain other physical quantities. Because it uses a random number initiator, computations can be completed in parallel. Therefore, the computation time is shorter. This paper will show in sequence the steps of this technique. The calculation begins by assigning a value to the incident energy and random position of the nucleons, and then ends after fission products occur. This paper only describes the process of calculating the Fission Yield for several U isotopes.

Keywords: Fission Yield, Semi Empirical, JENDL, Random Number.

INTRODUCTION

It is well known that fission yield data (FYD) are indispensable for some industries related to nuclear technology such as nuclear reactors and fuel cycle technology. In nuclear reactors, FYD is widely used to calculate fuel utilization, such as decay heat, dosimetry, reactor safety, burn-up, waste treatment, and so forth. The FYD mentioned in this paper is actually a secondary product of the fission process. This is because neutrons as primary products undergo evaporation in a very short range of time.

Since the discovery of fission reactions and their use in nuclear technology has emerged a large number of studies have been and are being carried out. One of the most important is research on fission yield products (FYP) in 1974. In that year, Moriyama and Ohnishi tried to approach the theory through a semi-empirical model [1]. As well as Katakura [2] he also did the same work with the semi-empirical approach. Based on the FYD experimental data, the Gaussian function was chosen to represent the data. For this purpose, Katakura had chosen five Gaussian functions. The parameters contained in the function were taken from the measurement results unless there was a parameter quoted from the work done by Wahl [3]. In another report [4], Wahl did a more complete elaboration of the calculation of physical quantities in the FYD systematic process. Danu [5], did the same thing as Moriyama in 2018 by using five Gaussian functions. He used experimental data and calculations by GEF [6] to get parameters in the Gaussian distribution function. In his paper, he considers that the isotopic yield followed a Gaussian distribution. The evidence that shows Gaussian-like functions are used as a function in semi-empirical methods can be seen in the work done by Lee [7]. Thus, FYD research that using the semi-empirical method can be said as continuing for more than 44 years, hence the method can be further developed.

Semi-Empirical Random Number Method for Fission Process (SERNM) is a semi-empirical method based on random numbers. This technique was developed based on the results of research conducted by Rizal [8-10]. According to Rizal, Fission reactions can be viewed as a stochastic process because the fission products cannot be determined with certainty only by one fission reaction. Based on this, many fission reactions are needed to find out. The recapitulation of all possible fission products will then form a value that can determine the probability of the emergence of a

1* Corresponding author.
E-mail address: rijalk@itb.ac.id

particular type of fission product. Unlike the model proposed by Brosa [11], the determination of this fission product does not use a potential barrier. So it has not been able to determine fission products from the results of fission. This condition is one of the weaknesses of SERNM.

THE METHOD

SERNM adopts the nucleus shape as in the liquid drop model. This technique divides the nucleus into two main parts, namely the left and the right. This division is a sign of the part that will experience fission. Furthermore, the generation of random numbers becomes the beginning of the simulation of fission events. The key to the success of SERNM is the use of random numbers, where this random number will determine the most likely nucleon distribution function. This distribution function can describe how nucleons are distributed in the nucleus when a fission event occurs. In order for the nucleon distribution to be more realistic, the chosen distribution function can follow the form of the nucleon distribution obtained from several sufficient references.

The nucleon distribution function according to Hofstadter [12] is in the form $\rho(r) = \rho_0\left(1+\frac{ar^2}{a_0^2}\right)exp\left(-\frac{r^2}{a_0^2}\right)$. The expression $exp\left(-\frac{r^2}{a_0^2}\right)$ has a Gaussian form. Wang [13] in his works states that the density of nucleons ^{120}Sn from experimental results can be approached by the sum of functions similar to Hofstadter. The next consideration was the work of Haddad [14]. He gave the result that the density of the charge on the nuclide narrowed in its centre.

The figure below shows an illustration of the relationship between nucleons and the intended Gaussian distribution function. This Gaussian function gives the probability that the nucleon lies around its mean position.

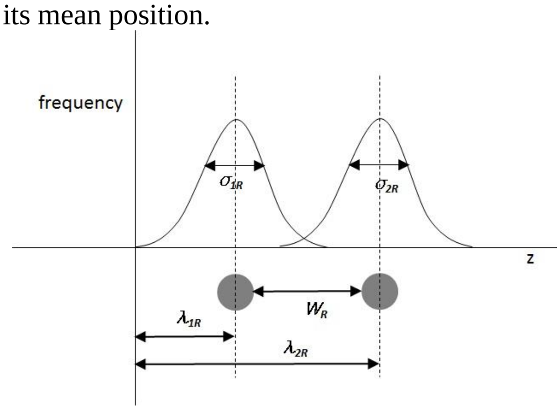


Fig. 1. Illustration of two Gaussian distribution functions representing the positions of two nucleons.

λ in Figure 1 shows the most likely nucleon position, while σ represents the width of the distribution function. The smaller the σ means the more the nucleons are bounded around the λ value. W is the distance between the two λ. The probability of the location of each nucleon is described in the following function.

$$f(z,\lambda_i) = B_i exp\left(\frac{-(z-\lambda_i)^2}{\sigma_i}\right) \quad (1)$$

With the explanation as follows: The scattered nucleons in the nucleus space are isotropic in the $x-y$ plane. Nucleons are only scattered following the z variable. z is a variable on the z-axis (see Figure 2), λ is a position where it has the greatest probability of finding the nucleon, and the standard deviation σ whereas i states the $i-th$ nucleon. Selection of the z-axis follows the illustration given by Nix [15].

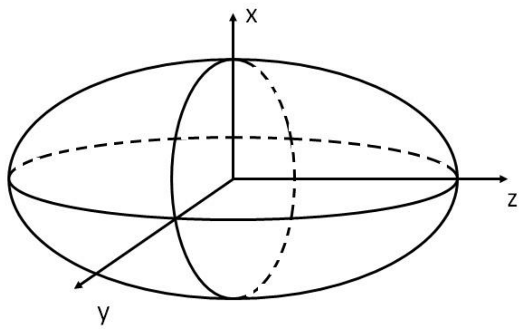


Fig. 2. Illustration of nuclear deformation in x-y-z space.

In SERNM, random numbers are used for two purposes. The first is to determine the ratio between the mean distance of nucleons on the right and the left. The second role is to determine the proportion between the width of the distribution function of the left and right nucleons. The following equation shows the use of these random numbers.

$$\xi_W = \frac{W_R}{W_L} \quad (2a)$$

$$\xi_\sigma = \frac{\sigma_R^{max}}{\sigma_L^{max}} \quad (2b)$$

For the distribution of the whole nucleon in nuclide that has mass number A, a superposition of equation 1 is applied to the whole nucleon in the nucleus.

$$F_j(z) = \sum_{i=1}^{A} B_i exp\left(\frac{-(z-\lambda_{ij})^2}{\sigma_{ij}}\right) \quad (3)$$

Equation 3 above will produce a distribution function that resembles the Fermi-Dirac distribution function. This equation is then called the Fermi-Dirac-like distribution function. With B_i is the normalization constant and,

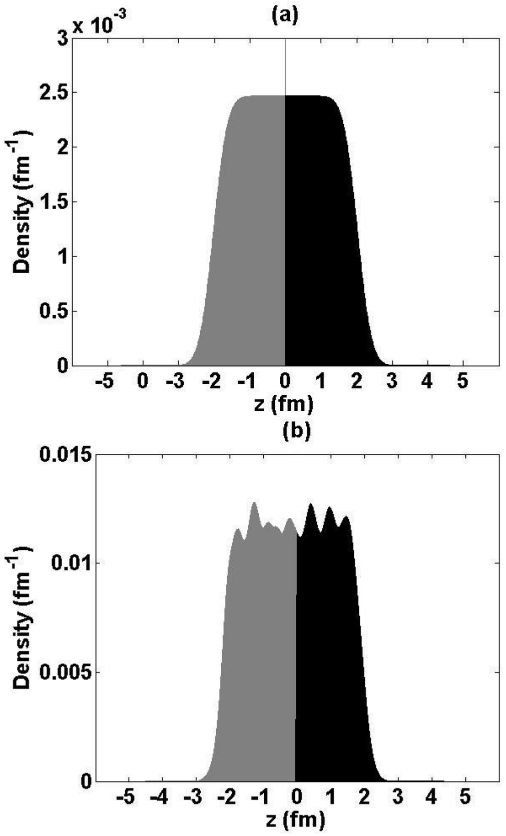
$$\lambda_{ij} = \{C_j - W_j, \dots C_j - W_j + kD_j^{\lambda}\}; \quad k = 1, \dots, A-1 \qquad (4)$$

$$D_j^{\lambda} = 2\frac{W_j}{A-1} \qquad (5)$$

C_j represents the centre of the future candidate fission nuclide with $j = \{L, R\}$ and L mean the left and R right parts of the candidates for fission nuclides. W_j is related to the total width of the distance between nucleons and D_j^{λ} denotes the average distance between nucleons. The width of the distribution function per nucleon σ_{ij} is,

$$\sigma_{ij} = \{\sigma_j^{min}, \dots \sigma_j^{min} + kD_j^{\sigma}, \dots \sigma_j^{max}\}; \quad k = 1, \dots, A-1 \qquad (6)$$

$$D_j^{\sigma} = \frac{\sigma_j^{max} - \sigma_j^{min}}{A-1} \qquad (7)$$



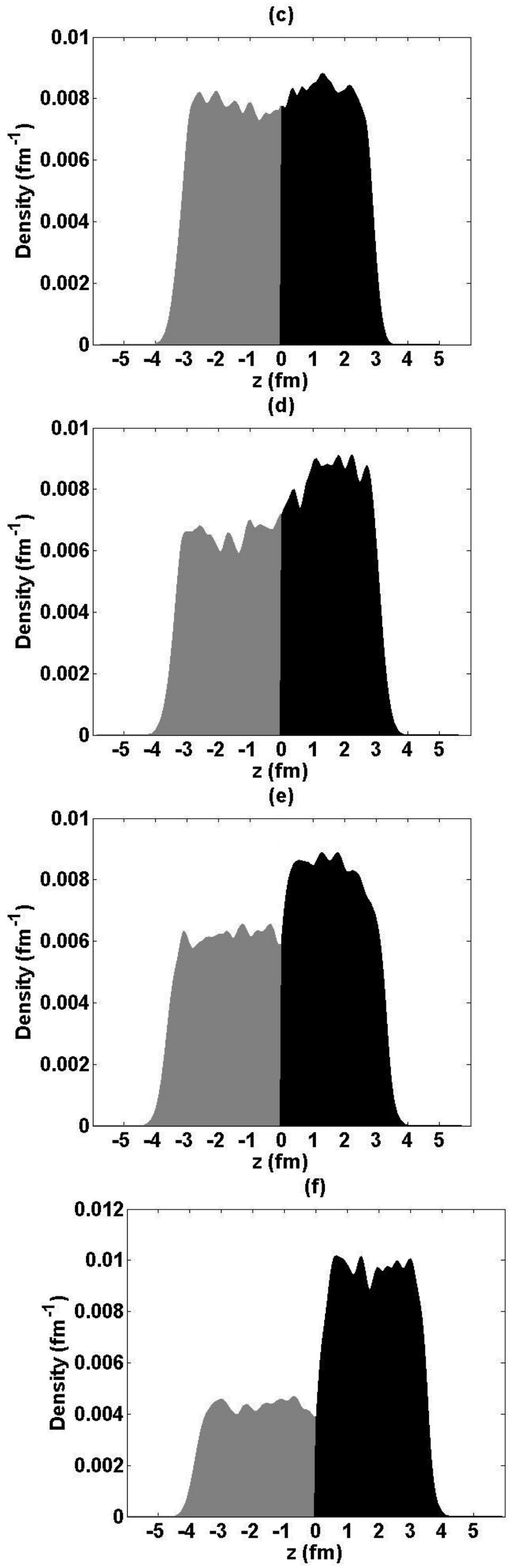


Fig. 1. These figures a→b→c→d→e→f Illustrate fission events by removing neutron prompts and delayed neutrons in this case

Figure 3 illustrates the fission events of the SERNM. The plot results of equation 3 can be seen in Figure 3(a). Picture (a) tells about the nucleus state before the fission process occurs. In this case, the nucleons are spread evenly in the undeformed nucleus. Figure 3(b) tells about the initial formation of a compound nucleus where the nucleons have different individual densities probability function. SERNM illustrates a nucleon as a density function (see equation 1). The energy received by the nucleus from outside causes the nucleons to change their position and density function shape. This event occurs as a result of energy changes from each nucleon. As a consequence, the density (it is built by equation 3) is no longer flat. Figure 3(c) starts to appear scattered alongside the z-axis. The image moves away from $z = 0$ and then the curve begins to decrease. Referring to Fink and Maruhn [16-17], the parameter C_j acts as a fragment coordinate. Due to the energy from outside the nucleus, this parameter enlarges to the maximum limit. The equation below describes the intended C_j change. χ is the SERNM parameter to be adjusted.

$$C_L^{new} = C_L^{old} - \chi; \quad C_R^{new} = C_R^{new} + \chi; \tag{8}$$

If it has reached the maximum stretching limit, the random numbers in equation 2 will contribute only to the nucleons spreading within the nucleus. This process is what happened to the image (d-e). Finally, picture (f) shows the processing of the nuclear rupture neck.

One iteration from the Figure 3(a) to 3(f) is called fission event. To determine the fission yield curve, it needs N fission event. As the principle in Monte Carlo, the greater the value of N causes the smaller random variation from calculation results. Therefore, it is necessary to generate as many random numbers as possible or as many as possible of fission event.

In Figure 3(f), equations 9 to 11 determine the left and right mass fractions.

$$A_L = \frac{I_L}{I_L+I_R}A; \;\; A_R = \frac{I_R}{I_L+I_R}A \tag{9}$$

$$I_L = \sum_{i=1}^{A} \frac{1}{2}\sqrt{\pi\sigma_{iL}}\left(1-erf\left(\frac{\lambda_{iL}}{\sigma_{iL}}\right)\right) \tag{10}$$

$$I_R = \sum_{i=1}^{A} \frac{1}{2}\sqrt{\pi\sigma_{iR}}\left(1-erf\left(\frac{\lambda_{iR}}{\sigma_{iR}}\right)\right) \tag{11}$$

The flow chart for the model is shown by Figure 4,

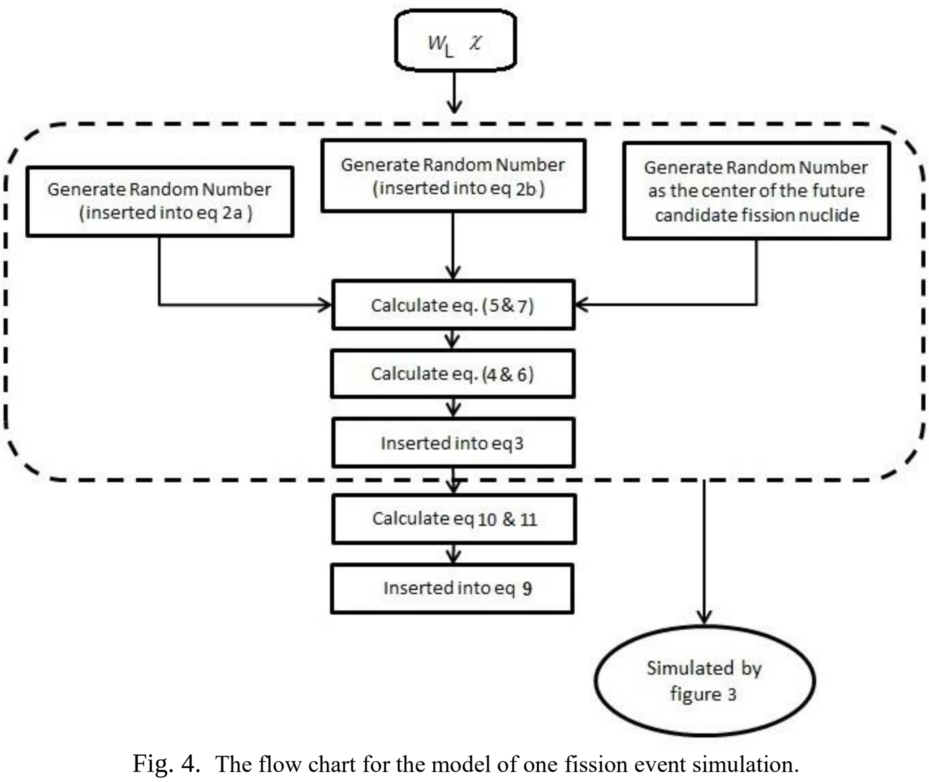


Fig. 4. The flow chart for the model of one fission event simulation.

Figure 3 illustrates the fission process. The flow diagram in Figure 4 explains the details of the process. Starting with generating a random number and then moving the parameter C_j according to equation 8. Continuously shifting until a thinning of the neck is reached and a break occurs. This fission process is called a fission event.

RESULTS AND DISCUSSION

SERNM is a semi-empirical method. Hence there are several parameters in the SERNM that are adjusted based on experimental data. They are W_L and χ . The process of matching these parameters uses fission yield experimental data. The resulting parameters are then used to determine other related physical quantities. One of the physical quantities referred to is the potential barrier peak on the nucleus deformation energy curve. In this paper, only SERNM parameters are presented.

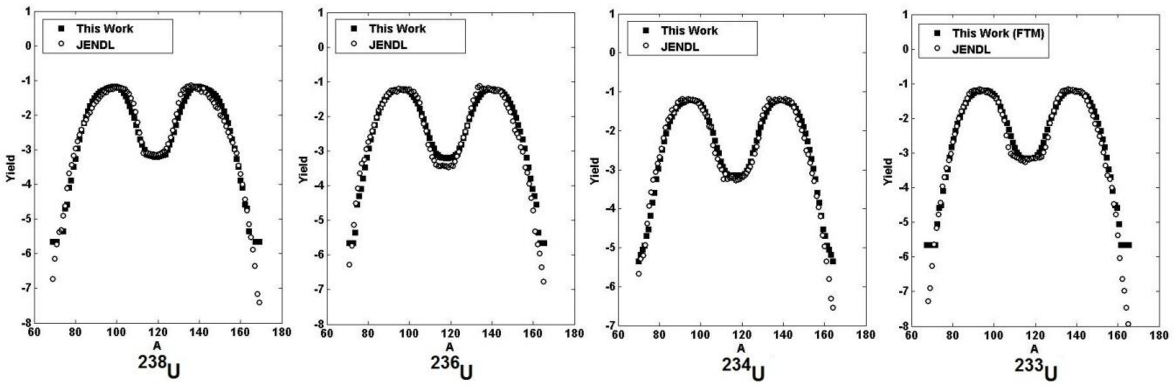


Fig. 5. Fission Yield of ^{238}U, ^{236}U, ^{234}U, ^{233}U with incident energy 500 keV

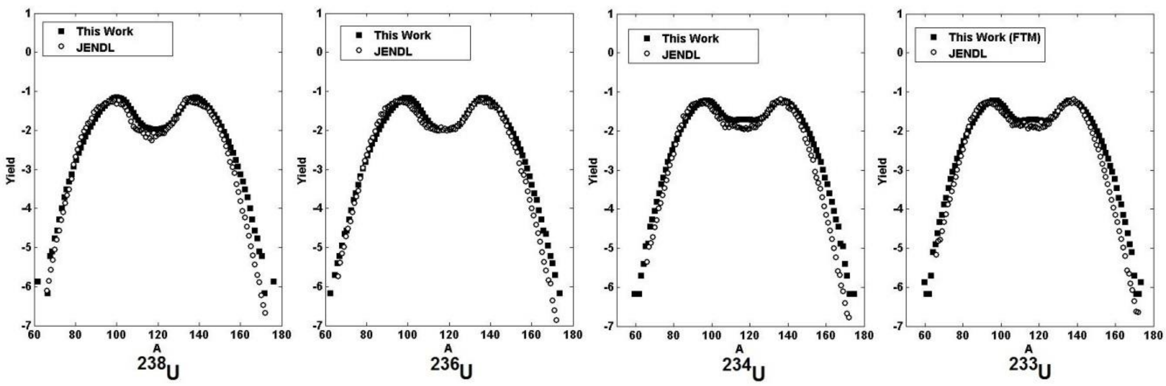


Fig. 6. Fission Yield of ^{238}U, ^{236}U, ^{234}U, ^{233}U with incident energy 14 MeV

The SERNM parameters used to produce Figure 5 are the same for all nuclides ^{238}U, ^{236}U, ^{234}U, and ^{233}U, the difference lies only in the value of A. It can be seen that the discrepancy between Calculation and JENDL are 3.9% for ^{233}U, 1.05% ^{234}U, 1.48% for ^{236}U and 3.9% for ^{238}U.

In general, the error between the results of the calculation by this method with the JENDL data is less than 11%, the majority less than 10%, which shows that the adjustment process was well done. The results of adjusting the data for 500 keV energy give W_L values of 50, 10, and 5 with weights of 1%, 69%, and 30%. Meanwhile, the incident energy for 14 Mev is 80, 20, and 5 with weights of 20%, 79%, and 1%. Both of these energies produce a χ value of 0.06.

What is the meaning of W_L = 80? Equation 5 can answer that question, if W_L inserted into equation 5, the distance between the nucleons will be about 0.6 fm. Refers to the nuclear radius, it estimated by $r_0A^{1/3}$, the maximum distance between nucleons is 2.4 fm. Thus, the value of W_L = 80 indicates that the nucleons are assembled and solidify about 4 times. When the value of W_L = 20, the nucleon density is solid about 14 times.

The configuration of the W_L weights illustrates the distribution of the W_L values at the nucleus that will be fission. Actually, the number of

W_L configurations can be selected more than three. The selection of the three W_L values is only for ease of comparison. For low energy of 0.5 MeV, the nucleons tend to congregate compared to an energy of 14 MeV. This is easy to understand; the incoming energy gives the nucleons the ability to scatter.

This semi-empirical method cannot distinguish between protons and neutrons so that for the same W_L and χ, the same fission yield for an isobar is produced. Therefore, further studies are needed to see the relationship between SERNM parameters with mass number, atomic number, and incident energy.

CONCLUSION

SERNM has successfully demonstrated its capabilities as a reliable semi-empirical method. The results of calculations using SERNM are the parameters W_L and χ. This parameter describes the response of the nucleon when it receives incoming energy. The response is the spread of the nucleons in the nucleus. Through SERNM, the deployment can provide information about the evolution of nuclear fission. This achievement makes the SERNM parameter useful for calculating several other related physical quantities. One of these physical quantities is nuclear deformation energy.

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