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The Dependence of the Rupture Probability on the Mass Number of the Fissionable Nucleus

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ABSTRACT

The relationship between the mass number of fissionable nuclei and fission yield is generally known through the fission barrier. The deformation energy of the SEMF determines the probability of the formation of fission products. The use of deformation energy is very impractical because it goes through many calculation stages. For this reason, the Neck Rupture Model was introduced, namely a model that shortens the stages of the calculation process through the rupture probability formula. In this paper, a new technique was introduced that adds the dependence of the rupture probability on the mass number of the nucleus that will undergo fission. Apart from this, this technique also obtained better fission yield calculation data compared to the previous technique. The fission yield calculations of Uranium isotopes at an energy of 14 MeV will be shown.

INTRODUCTION

The atomic nucleus is a quantum system of protons and neutrons held together by a strong nuclear force. Under certain conditions, the nucleus can split into two or three fragments and decompose by emitting particles. This phenomenon is called nuclear fission [1]. This topic needs to be studied, considering that nuclear technology has become dominant for human civilization. Nuclear power plants and batteries are among the most advanced and valuable uses of nuclear technology. Therefore, understanding nuclear reactions is essential and must be studied carefully. Fission yield is one category that describes nuclear fission, commonly called fission product properties. Fission yield is the portion of how many fission fragments formed in a nuclear fission reaction and the portion of the distribution of the types of fission fragments formed. Knowing the fission yield can more easily manage fission waste and maintain the safety and optimization of nuclear reactors. To understand more about this nuclear fission reaction, including its fission yield, researchers developed many software programs, and TALYS is one of them.

The idea for creating TALYS was born in 1998 at CEA Bruyères-le-Châtel, France. TALYS is a computational tool that combines theoretical models and experimental data. The software uses the FORTRAN programming language. By entering relevant parameters into TALYS, we can predict experimental results, especially those that cannot be obtained through laboratory results. TALYS works by simulating the interaction between a nuclear target and its projectile. TALYS is renowned for its accuracy and ongoing improvements that researchers continuously develop. On December 30, 2021, TALYS code released a new version, TALYS 1.96. [2]. Unfortunately, the fission data calculation results are not yet close to the evaluated nuclear data. Therefore, the author will modify the TALYS code in this section using the Brosa model.

The Brosa model is used in the TALYS code to analyze fission results [3]. The Brosa model was proposed by Ulrich Brosa and his colleagues in 1990 [4,5]; this model is called the Random Neck Rupture Model (RNRM). RNRM is a calculation of post-fission observations such as mass distribution, kinetic energy distribution, and neutron multiplicity.

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According to this model, the pre-fission shape of the fissionable nucleus determines the post-fission observations. One of its successes is explaining the wide distribution of mass in low- and medium-energy fissions [6]. Therefore, we will improve and modify the Brosa model for high-energy fission reactions. Due to the need for more accuracy in the calculation results of the TALYS software, which uses the Brosa formulation to calculate the probability of fission at high energies, modifications were made to the Brosa formulation. Uranium nuclides were tested for modifications made to achieve nearly identical nuclide properties.

THEORY

Fission yield or mass distribution of fission fragments is the number and type of particles released when an atomic nucleus splits or undergoes nuclear fission. In general, normalized fission yield can be expressed in the following Eq. (1).

$$Y(A_{FF}) = \sum_{FM}[W_{FM}.Y_{FM}(A_{FF})] \tag{1}$$

FM is a fission mode consisting of super long (SL), Standard I (ST-I), and Standard II (ST-II). Meanwhile, A_{FF} is the mass number of the nuclide resulting from fission, see Eq. (2).

$$W_{SL} = \frac{T_{SL}}{T_{SL}+T_{ST-I}+T_{ST-II}} \tag{2}$$

With,

$$T_{FM} = \int_0^{\infty} \rho_{GS}\left(1 + exp\left(\frac{2\pi B_{FM}+\varepsilon+E_X}{\hbar\omega_{FM}}\right)\right)^{-1} d\varepsilon \tag{3}$$

ρ_{GS} is the energy density in the ground state, E_X is the achieved excitation energy, B_{FM} is the barrier height of the deformation energy potential, and $\hbar\omega_{FM}$ is the potential width of the deformation energy as provided in Eq. (3). For the present, the fission yield of each fission mode is determined by using Eq. (4) as follows.

$$Y_{FM}(A_{FF}) = y(A_{FF}) + y(A - A_{FF}) \tag{4}$$

A is the mass number of the nucleus that will fission, while the following Eq. (5) expresses y,

$$y(A_{FF}) = exp\left(-\frac{2\pi\gamma_0\left(\rho^2(z_r,A_{FF})-\rho^2(z,A_{FF})\right)}{T}\right) \tag{5}$$

γ_0 is related to the surface tension constant in the Liquid Drop Model- LDM [7], and $\rho(z)$ is the surface distance to the z-axis in the LDM form, while T is the temperature. The index *r* on z refers to the rupture model [8].

METHODOLOGY

According to the Liquid Drop theory, the surface energy model is determined by the formula $E = \gamma\Delta A_S$, where A_S is the surface area of a nuclide. It is highly dependent on the number of nucleons, namely the mass number (A). TALYS takes an approach by using surface energy as a physical quantity in the partition function $Z = exp(-E/T)$. TALYS chooses this by assuming that the contribution of surface energy dominates the fission process. The fission process is a complex system. The fission barrier that is formed not only depends on the surface energy but also depends on macro- and micro-events; hence, corrections to the surface energy are necessary. This correction factor can be a function that is multiplied by the surface energy. Thus, the correction factor for Eq. (5) in TALYS has a value of 1. For simple correction, a correction factor is tried in the form of a number that is not 1. Furthermore, this correction factor is introduced as V_{nuk}.

The TALYS code was then updated. The first step is to locate and identify the section of code that represents the rupture probability formula. Therefore, $P(A)$ is added to a specific line in the TALYS library in the form V_{nuk}. After TALYS was modified, an experiment was conducted to determine whether the fission yield graph improved or worsened, referring to the evaluated nuclear data by entering any V_{nuk} value. The following regression was carried out to compare the estimated nuclear data with the data provided by TALYS.

The maximum regression coefficient (R^2) value can be obtained by using the V_{nuk} value as the independent variable on the x-axis, with the R^2value as the dependent variable on the y-axis. The highest R^2 value that gives the desired V_{nuk} value. This process is repeated for different mass numbers but remains in one isotope. The results obtained from this repetition are then approximated by the polynomial $P(A)$ in Eq. (6).

$$y(A_{FF},A) = exp\left(-P(A)\frac{2\pi\gamma_0\left(\rho^2(z_r,A_{FF})-\rho^2(z,A_{FF})\right)}{T}\right) \tag{6}$$

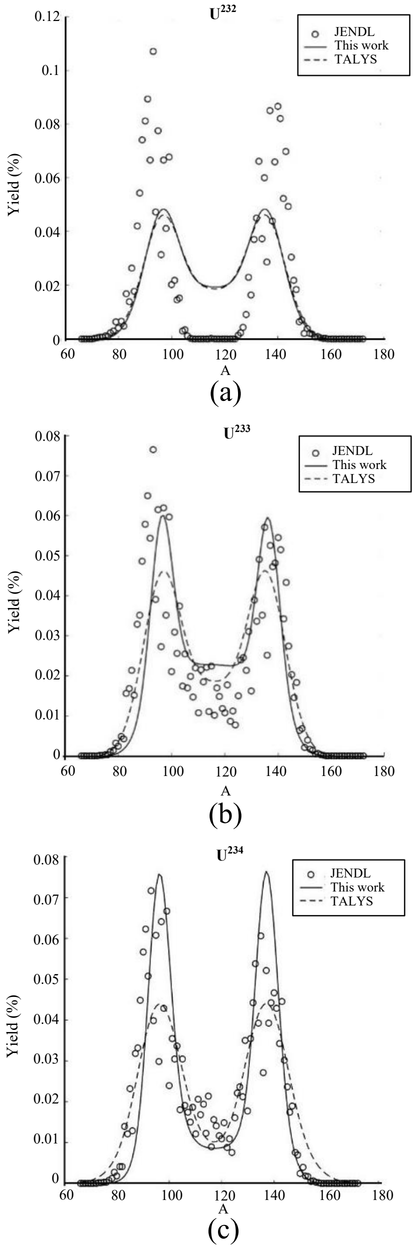
Here is a modified code snippet from TALYS' neck.f as depicted in Fig. 1. Modifications were made to line 293 of the neck.f file by adding the variable “Poly”.

```
290            eob=2.*pi*gam*(rhodi(zriss)**2-rhodi(z2)**2)
291            wgt(jmx)=0.
292            expo=eob/tmp
293            if(expo.lt.80.) wgt(jmx)=exp(-Poly*expo)
294            af1(jmx)=am1
295            zf1(jmx,izloop)=ze1
296            af2(jmx)=am2
297            zf2(jmx,izloop)=ze2
298      4     continue
299      3     continue
300            jimax=jmx
```

Fig. 1. Modified TALYS neck.f snippet.

RESULTS AND DISCUSSION

Calculations have been carried out for 7 Uranium isotope nuclides, namely U^{232}, U^{233}, U^{234}, U^{235}, U^{236}, U^{237}, U^{238}. The calculation results through modification of Eq. (5) are shown in Figs. 2 (a-g).



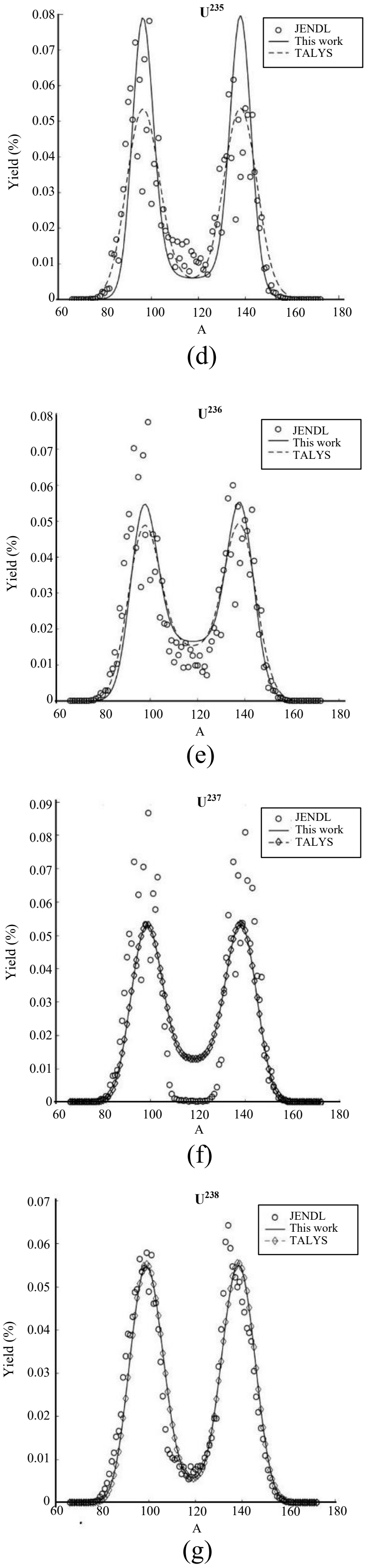


Fig. 2. Fission yield of Uranium Isotopes such as (a)U^{232}, (b) U^{233}, (c) U^{234}, (d) U^{235}, (e) U^{236}, (f) U^{237}, and (g) U^{238} at 14 MeV energy.

Although the analysis was carried out qualitatively, namely visually, these images clearly show the differences and similarities between TALYS, this technique, and JENDL.

In Figs. 2 (a-g), it can be seen that the results of TALYS and this study have succeeded in approaching the JENDL value for the U^{238} fission event and have discrepancies for U^{232}. At U^{232}, U^{237}, and U^{238}, TALYS and the results of this work have values that can be said to be similar. For the fission events, the U isotopes do not have symmetric fission products, even though in the fission of U^{238}, TALYS and this work still show small discrepancies with JENDL. This is because the dominance of symmetric products is generally produced by reactions at fairly high energies. For 14 MeV, the energy is still not enough to produce symmetric fission products. In other words, the similarity of results between TALYS and this work is unrelated to whether the fission products are symmetric or not. However, this technique can predict every fission with asymmetric fission products better.

At U^{233}, U^{234}, and U^{235}, TALYS is consistently lower than the results of this polynomial addition technique. This condition is possible due to peak sharpening in Eq. (6). The addition factor $P(A)$ will automatically increase the maximum value of both fission product peaks. This technique is the main correction factor in the formulation of TALYS.

Adding parameters to Eq. (6) will affect the fission yield calculation, specifically for asymmetric fission products. Generally, the parameter value of Eq. (6) is smaller than 1; this condition indicates that the fission product pattern will narrow around its highest value. The TALYS pattern is more sloping. The symmetrical product area will automatically thicken by reducing or sharpening the pattern. Figure 2 (b) shows thickened symmetric areas.

Approximation of a function through a polynomial is commonly used in the curve-fitting process. A curve-fitting process was carried out to see the relationship between this $P(A)$ (Eq. (7)) and the mass number undergoing fission. The polynomial is similar to SEMF (Semi-Empirical Mass Formula) [9].

$$P(A) = a.A + b.A^{2/3} + c.\left(\frac{Z(Z-1)}{A^{1/3}}\right) + d.\frac{(A-2Z)^2}{A} + e.A^{-3/4} \quad (7)$$

Where Z is the atomic number.

The fitting results provide the following coefficient values: a = -14.236, b = 18.3868, c = 0.8114, d = 20.0892, e = -19.9493. An error of around 10 % is sufficient to ensure there is a close statistical correlation. These coefficients can be close to the coefficient values of SEMF. The choice of this polynomial is to show that the formula in Eq. (6) is related to the nuclear deformation energy according to [10,11], SEMF is the foundation of forming binding energy. Thus, it will directly affect the formation of deformation energy.

For high energies, symmetric fission products generally dominate. The energy of 14 MeV is included in the beginning of the high energy range, so naturally, $P(A)$ is smaller than 1. These conditions indicate that fission product data distribution will narrow around the highest value and stack or thicken in the symmetric area.

Deformation energy is a barrier that must be crossed when a nuclide system experiences excitation [12]. The nuclide state tends not to oscillate for high energies because it has almost passed the potential barrier. These conditions indicate that there will be variations in fission products that are practically homogeneous. So, the fission yield curve will not have two peaks, but a plateau will form.

Based on the explanation that has been presented, it is perfect if it is approximated by a polynomial that resembles the deformation energy.

The deviations shown in Fig. 2 can be seen as limitations of this technique and TALYS. These two calculations cannot handle the occurrence of successive fission reactions, which is known as the cascade model [13-15]. Consecutive fission events cause the distribution to become more spread out. Consequently, the fission yield curve forms two sharp peaks without any areas for symmetric products.

The cascade model is a reaction model that involves a multi-stage process, meaning that the target hit by the projectile will undergo a series of fission events. This multi-stage event has consequences for the fission products obtained. The recorded fission products will be more varied compared to single-stage fission reactions. Experimental data, of course, are data resulting from multi-stage events. Since JENDL is evaluated data from experimental results, JENDL data is automatically multi-stage data. As mentioned, this calculation technique is a single-stage model, meaning that the results obtained do not approach JENDL data.

CONCLUSION

Using polynomials (7) in Eq. (5) provides more accurate fission yield calculation results than without insertion. Apart from that, the insertion of this polynomial can sharpen the meaning of the dependence of the fission probability on the nuclear binding energy. Nuclear binding energy, which was previously only helpful in determining the opportunity for fission to occur, now plays a more visible role as one of the determining components for forming fission products.

By complementing the various nuclides that exist, the role of the polynomial will likely appear more clearly.

Based on the results obtained from this research, further attempts will be made to apply to other elements and other energy ranges as long as the data is still available.

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AUTHOR CONTRIBUTION

Z. Auliya and R. Kurniadi equally contributed as the main contributors of this paper. All authors read and approved the final version of the paper.

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