Modified Boltzmann Factor on Rupture Probability

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Abstract

Fission Products are data that is very much needed for developing nuclear technology. Considering that the experimental results of nuclear data are minimal, theoretical modeling and calculations are needed. One of the theoretical models is the "multimodal random neck-rupture model. (M-RNRM)" However, although it has completed the fission product data, it needs closer to the reference value. For this reason, the idea of modifying the Boltzmann factor on rupture probability was developed. This modification is in the form of adding a polynomial factor to the Boltzmann factor. This work has succeeded in showing better fission product calculation results closer to the reference value.

Keywords: Fission Product, Theoretical Model, M-RNRM, Boltzmann Factor.

INTRODUCTION

Nuclear data is a collection of information related to nuclear reactions. Nuclear data can be cross-sections, fission products, decay constants, energy levels, or energy spectra. For the application of nuclear reactors, the indispensable data for nuclear data are cross sections and fission products [1]. Given the importance of fission product data, several semi-empirical and theoretical models have been developed, such as microscopic and macroscopic models. TALYS is software that applies several models and methods to obtain nuclear data [2]. TALYS chose the "Temperature-time dependent Brossa Model" as the primary formulation in determining the physical quantities of the distribution of fission products. The formulation was based on the "multimodal random neck-rupture model" (MM-RNMM) [3,4].

This model is composed of two interconnected components: the multi-channel evolution towards scission and the utilization of RNRM after scission. These two components complement each other so that a yield value that has properties analogous to the experimental results can be produced [5].

An excited nucleus will deform into specific forms. The path that passes is a 6-dimensional space that contains the parameters of the shape of the deformation. Of course, the path chosen is the path with the lowest energy. The final form of the nuclide before scission is a vast, flat neck. This shape is called pre-scission. According to Niday [6] and Brossa [7], this channel is composed of three main channels, namely standard I (ST-I), standard II (ST-II), and superlong (SL). Even though it is unlikely to appear, supershort (SS) is one of the channels that can be involved.

The search for fission channel modes is carried out by minimizing the surface energy potential. The surface energy potential is obtained due to the deformation of the fissionable surface of the core. In this calculation, PES is affected by temperature, so the formulation depends on free energy. The addition of the effect of temperature is increasingly seen in changes in the shape of the fission barrier curve and the excitation energy. The PES model is the model proposed by Strutinsky [8]. The shape of the core deformation greatly influences PES, for the shape of the core deformation refers to the standard form of Lawrence [9].

Furthermore, this Lawrence form is used together with the total energy of the nucleus through the liquid drop model (LDM) [10]. When the nuclide is excited, the volume and surface area increase while the density and surface tension decrease. This phenomenon has been observed by Hasse[11]. This volume increase ends upon entering precision. According to Brosa, the probability of

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rupture follows the Boltzmann factor formulation. This probability is then helpful for calculating the desired fission product. The modeling results used by TALYS are still far from the JENDL data. Therefore, this work proposes an alternative modification of the Boltzmann factor by adding a polynomial to the exponential.

THE METHOD

As has been reviewed in the introduction, our focus is on the modification of the Boltzmann factor. For this reason, discussing the components involved in the formulation is better. The discussion begins with the determination of the total energy of the nucleus.

The total energy of the nucleus follows the semi-empirical mass formula [11] E_{LDM}.

$$E_{LDM} = -a_1 \left[1 - \kappa \left(\frac{N-Z}{A}\right)^2\right] A + a_2 \left[1 - \kappa \left(\frac{N-Z}{A}\right)^2\right] A^{2/3} + \frac{3e^2 Z^2}{5 r_o A^{1/3}} + \frac{(\pi e d Z)^2}{2 r_o^3 A} \tag{1}$$

With $a_1 = 15.494 \ MeV$, $a_2 = 17.949 \ MeV$, $\kappa = 1.783 \ MeV$, and $r_o = 1.225 \ fm$

Then added the effect of temperature so that thermally defined as:

$$F(T) = E(T) - TS \tag{2}$$

T is in MeV units, and S is in MeV/K units. The assumption used is that the system is in an isothermal state.

$$n(T) = n(0)(1 - 0.0032T^2)$$

$$\sigma(T) = \sigma(0)(1 - 0.0114T^2) \tag{3}$$

Through these equations of density $n(T)$ and surface tension $\sigma(T)$, the energy volume, surface, and coulomb are then obtained.

$$F_{vol}^{LDM} = E_{vol}^{LDM}(0)(1 - 0.0032T^2) \tag{4}$$

$$F_{surf}^{LDM} = E_{surf}^{LDM}(0)(1 - 0.0012T^2) \tag{5}$$

$$F_{coul}^{LDM} = E_{coul}^{LDM}(0)(1 - 0.0010T^2) \tag{6}$$

Finally, the Free Energy formulation from LDM was formed.

$$F_{def}^{LDM} = F_{surf}^{LDM} + F_{coul}^{LDM} \tag{7}$$

Strutinsky's formulation requires a complete set of energy levels for skin correction. These energy levels are obtained through various potential models and desired core models. In TALYS, the model chosen is the BCS model [12]. The Hamiltonian used is:

$$H_n = \frac{p^2}{2m_n} + V_n(r) - \frac{\lambda}{2(m_n c)^2} \boldsymbol{s}.\left[\nabla V_n(r) \times \boldsymbol{p}\right] \tag{5}$$

$$H_p = \frac{p^2}{2m_p} + V_p(r) - \frac{\lambda}{2(m_p c)^2} \boldsymbol{s}.\left[\nabla V_p(r) \times \boldsymbol{p}\right] + V_{coul}(r) \tag{6}$$

$$V_{n,p} = \frac{V_{0,np}}{1 + exp\left[\frac{\rho - R}{\alpha}\right]} \tag{7}$$

While the potential chosen is the potential of Wood-Saxon [13].

R and α are nuclear radius and diffuseness respectively. Thus the energy and entropy of the system become,

$$E^{BCS} = \sum_{k>0}^N \epsilon_k \left[1 - \frac{\epsilon_k - \lambda_F}{\epsilon_{qp}} tanh\left(\frac{\epsilon_{qp}}{2T}\right)\right] - \frac{\Delta^2}{G} \tag{8}$$

$$S^{BCS} = 2\sum_{k>0}^N \left(ln\left(1 + exp\left(-\frac{\epsilon_{qp}}{T}\right)\right) + \frac{\epsilon_k}{T(1 + exp(\epsilon_k))}\right) \tag{9}$$

The solution to the equation of state Equation 7 gives the temperature values.

$$T(\epsilon) = \sqrt{\frac{\epsilon}{a_{gs}}} \qquad (10)$$

The value of a_{gs} is obtained through the equation below in the ground state.

$$a = \bar{a}\left(1 + \delta\frac{(1-\exp{(-\eta\epsilon)})}{\epsilon}\right) \qquad (11)$$

$\bar{a}$ is the level density parameter. Where its parameter does not use Strutinsky skin correction. The temperature formulation in Equation 10 is used to calculate the rupture probability.

$$\rho(\xi) = \begin{cases} (r_1^2 - \xi^2)^{1/2} & -r_1 \le \xi \le \xi_1 \\ r + \beta^2 c\left(cosh\left(\frac{\xi - z + l - r_1}{\beta}\right) - 1\right) & \xi_1 \le \xi \le \xi_2 \\ (r_2^2 - (2l - r_1 - r_2 - \xi)^2)^{1/2} & \xi_2 \le \xi \le 2l - r_1 \end{cases} \qquad (14)$$

In this work, the modification made is by adding a polynomial to equation 13. So that the form of equation 13 becomes.

$$W(A) \propto exp\left(-P(A_{CN})\frac{2\pi\gamma\left(\rho^2(z_r) - \rho^2(z)\right)}{T}\right) \qquad (14)$$

$$W(A) \propto exp\left(-\frac{E(z_r) - E(z)}{T}\right) \qquad (12)$$

The values of z and z_r are locations with a high probability of breaking and random places around the neck. When rupture occurs, the energy in Equation 12 is dominated by surface tension energy. Therefore this equation can be approximated by the following equation.

$$W(A) \propto exp\left(-\frac{2\pi\gamma\left(\rho^2(z_r) - \rho^2(z)\right)}{T}\right) \qquad (13)$$

The value of ρ is obtained by parameterizing the form of Lawrence.

variable ν. This variable would limit the search scope for the desired polynomial.

$$W(A) \propto exp\left(-\nu\frac{2\pi\gamma\left(\rho^2(z_r) - \rho^2(z)\right)}{T}\right) \qquad (15)$$

Table 1 shows the value of ν, which gives the most significant regression coefficient. To see whether this modification is reasonable, we can see the comparison with the regression coefficient of TALYS.

RESULTS AND DISCUSSION

JENDL is a compilation of evaluated nuclear data that provides various types of nuclear reaction data, one of which is fission products. This fission product data refers to data from ENDF. This JENDL has also been adapted to the decay data used in calculating the heat in the reactor [14]. The light ternary fission product owned by JENDL was obtained from the results of a fusion between the compilations from Rider [15] and Mills [16]. These two fission products combine to form a cumulative fission product. The data from JENDL is used as benchmarking to get the appropriate polynomial function.

Before starting the search for the polynomial that matches equation 14, we approach it with a

Table 1. The value of ν is used so that the calculation of fission products is close to the value of JENDL [17]

Nuclides	ν	R^2	R^2 TALYS
^{233}U	0.38	0.867	0.642
^{234}U	0.48	0.837	0.718
^{235}U	0.84	0.843	0.837
^{236}U	0.8	0.861	0.851
^{237}U	0.91	0.878	0.877

Nuclides	Linear	Quadratic	R^2 TALYS
^{238}U	0.78	0.896	0.884
^{238}Pu	1.5	0.833	0.807
^{239}Pu	2.07	0.832	0.759
^{240}Pu	1.72	0.860	0.815
^{241}Pu	0.94	0.810	0.810
^{242}Pu	0.74	0.841	0.824
^{242}Cm	2.72	0.846	0.718
^{243}Cm	1.73	0.796	0.764
^{244}Cm	1.55	0.841	0.812
^{246}Cm	1.55	0.866	0.836
^{248}Cm	1.98	0.826	0.758

The numbers in the table show that adding the ν parameter value gives a better regression coefficient value than TALYS. The better deal of the regression coefficient indicates that this modification can provide a closer fission product compared to TALYS.

If we look closely, there is a pattern between the value of ν and the mass number of the nuclide. These values indicate a correlation between the value of ν and the mass number for that done curve fitting.

Two types of polynomials are used in this work, namely linear and quadratic. The following is the result of the curve fitting for Uranium :

$$\nu(A) = 0.093A - 21.17 \qquad (16)$$

$$\nu(A) = -0.04A^2 + 18.176A - 2150 \quad (17)$$

Table 2. The value of R^2 Uranium

Nuclides	Linear	Quadratic	R^2 TALYS
^{233}U	0.86	0.86	0.642
^{234}U	0.83	0.83	0.718
^{235}U	0.83	0.84	0.837
^{236}U	0.84	0.86	0.851
^{237}U	0.88	0.88	0.877
^{238}U	0.89	0.90	0.884

The curve fitting for Plutonium :

$$\nu(A) = -0.265A + 65 \qquad (18)$$

$$\nu(A) = -0.14A^2 + 67.36A - 8040 \quad (19)$$

Table 3. The value of R^2 Plutonium

Nuclides	Linear	Quadratic	R^2 TALYS
^{238}Pu	0.82	0.83	0.807
^{239}Pu	0.82	0.83	0.759
^{240}Pu	0.85	0.84	0.815
^{241}Pu	0.8	0.8	0.810
^{242}Pu	0.84	0.83	0.824

The following is the result of the curve fitting for Curium :

$$\nu(A) = -0.08A + 21.6 \qquad (20)$$

$$\nu(A) = -0.1A^2 - 50.9A + 6244 \qquad (21)$$

Table 4. The value of R^2 Curium

Nuclides	Linear	Quadratic	R^2 TALYS
^{242}Cm	0.84	0.845	0.718
^{243}Cm	0.8	0.8	0.764
^{244}Cm	0.83	0.84	0.812
^{246}Cm	0.84	0.85	0.836
^{248}Cm	0.82	0.83	0.758

All tables show that the quadratic form of the value of A to ν gives a more significant regression coefficient. Adding the ν parameter in equation 15 indicates that the relationship between rupture probability and the Boltzmann form is not linear. In other words, the total energy distribution of the nucleus cannot be viewed as a Boltzmann statistical distribution. This situation reinforces the fact that nucleons are fermions, so nucleons are fermions as well.

CONCLUSION

This work provides two critical conclusions.

First: The Boltzman factor in the rupture probability formulation needs to be modified so that the calculation results are closer to reference data such as JENDL.

Second: The addition of the polynomial to the Boltzmann factor emphasizes that the actual nuclide energy cannot be seen as a classical energy distribution. The energy distribution of fissionable nuclides must apply the Fermi Dirac distribution.

In addition, other aspects can be tested to strengthen the conclusions drawn by calculating the yield on the heaviest fragments and the fission barrier of several nuclides.

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