Model Calculation of Fission Product Yields Data using GEF Code

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1. Introduction

Fission product yields data play an important role in the nuclear industry such as prediction of decay heat, design of nuclear reactors and handling of spent fuel. Moreover, fission product yields data are closely connected nuclear safety and thus interest in it is recently growing more and more.

Fission yields data are classified with spontaneous fission data and neutron induced fission data. The fission product yields data at several energy points for the limited actinides are included in nuclear data libraries such as ENDF/B, JEFF and JENDL because production of those is based mainly on experimental results and it is very difficult to conduct experiments for all actinides and continuous energies. Therefore, in order to obtain fission yields data without experimental data, a theoretical fission model should be introduced to produce the yields data.

GEneral Fission model (GEF) is developed to predict the properties for fissioning systems that have not been measured and that are not accessible to experiment [1]. In this study, the fission yields data generated from GEF code are compared with the measured data and the recently available nuclear data libraries.

2. Theoretical Concepts in GEF Code

GEF code has accepted relatively new concepts in nuclear physics as well as several well-known ones [1, 2]. GEF code is written in FreeBASIC and calculates the fission properties with Monte Calro method. GEF code includes many ideas for model calculation. In this section, several concepts playing an important role in GEF code are described.

2.1 Separability principle

It is still challengeable to explain fission process only with theory because it is not fully understood yet. However obtaining experimental data of all nuclide and energy are also impossible. To resolve this problem, the macro-microscopic approach has been applied.

In the fission process, macroscopic potential on the fission path is specific to the fissioning system while shell effects on the fission path are associated to the nascent fragments [3].

Due to the separability principle, broad range of nuclear fission process could be calculated with this model which is based on empirical parameters.



Fig. 1. Potential energy for ²³⁸U fission [4]. (a) shows only macroscopic aspect (liquid-drop potential) whereas macroscopic-microscopic potential is expressed on (b).

2.2 Even-odd effect

Even-odd effect is a noticeable phenomenon which occurs in the charge distribution of fission product [5]. In the fission process, the fragments tend to be even-Z nuclide. This tendency can be explained to the parameter δ_p [6].

$$\delta_p = \frac{1}{8} (-1)^z [\ln Y(Z+3) - \ln Y(Z) - 3(\ln Y(Z+2) - \ln Y(Z+1))] \quad (1)$$

The δ_p decreases when mass of the fissioning system increases while it increases with asymmetry of fissioning nucleus [6]. GEF code contains a schematic model about even-odd effect.

2.3 Energy sorting

Energy sorting is the thermodynamic concept in fission process. It means that the hotter light fragment transfers almost all its intrinsic excitation energy to the colder heavy fragment [2]. This effect can be confirmed from the measurement of prompt-neutron yield. Figure 2 shows the prompt neutron yield of ²³⁷Np for 0.8 MeV and 5.55 MeV energy of incident neutron. The additional initial energy leads to an increased neutron yield from the heavy fragments, only. The relation between incident neutron energy and prompt neutron yield is well reproduced by the GEF code.

Besides prompt neutron yield, the idea of energy sorting is related to various concepts in GEF code such as excitation energy of the fission fragments and evenodd effect.



Fig. 2. Measured mean prompt neutrons yield of ²³⁷NP fission [7]. Prompt neutron yields are almost same for light fragment without reference to the incident neutron energy. However, heavy fragments show the difference in prompt neutron yield.

3. Comparison with existing data

Although GEF code includes various physical ideas such as fission process, thermodynamics and nuclear shell model, it also exploits systematics to reflect the phenomena of real world and fit the output of GEF in measured value. In this section, the results of GEF code were compared with experimental data and existing nuclear data libraries to check whether model calculation is reliable or not.

3.1 Calculation method

As input data, GEF code requires enhancement factor as well as target nucleus, fission type, incident neutron energy and so on. Enhancement factor decides event number of Monte-Calro simulation. In this study, 10⁶ events are calculated. The same event number is being applied to GEFY which is GEF-based fission-fragment yield library in ENDF-format.²³⁵U is selected as target nuclide because of its importance in nuclear industry and huge amounts of experimental data. In order to compare GEF with ENDF/B-VII.1, JEFF-3.1.1 and JENDL/FPY-2011, incident neutron energies are selected as 0.0253 eV, 400 keV, 500 keV and 14 MeV. Only independent yields are considered because GEF code doesn't have any decay information.

3.2 Comparison with experimental data

Because experimental data rarely contains comprehensive information, it should be handled carefully. In order to compare the measured data with the results of GEF code, scale change should be considered. GEF code gives fission yields which are normalized to 200. In other hand, the experimental data usually provide the number of produced nuclides per 100 fissions. In this study, sum of nuclide yields from experiment is adjusted to fit yields sum of same nuclides generated from GEF code. Experimental data of ²³⁵U fission are taken from EXFOR (Experimental Nuclear Reaction Data).

The mass distributions of thermal neutron (0.0253 eV) induced fission are shown in figure 3 for linear and log scale. Although fission yield of each mass number is not exactly same, GEF code successfully anticipates the location of peak and general shape of mass distribution.



Fig. 3. Comparison of experimental fission fragment mass distribution with the result of GEF code for linear and logarithmic scale.

Figure 3 shows that GEF code overestimates nuclide yields near peak while it underestimates off-peak nuclide yields. This tendency occurs equally when GEF results are compared with recently available nuclear data libraries. Even though nuclides in low yields may not play a significant role in fission process, there is a necessity for improvement.

	Exper	iment	GEF code		
nuclide	(W. Lang)				
	yield	error	yield	error	
⁹⁴ Sr	4.541	0.129	5.136	0.327	
¹⁰⁰ Zr	4.541	0.209	4.466	0.332	
⁹⁰ Kr	4.472	0.120	3.964	0.182	
⁹⁵ Sr	4.362	0.110	4.811	0.356	
⁹⁹ Zr	3.904	0.120	3.950	0.230	
⁹⁶ Sr	3.526	0.110	4.251	0.559	
⁸⁹ Kr	3.467	0.094	2.981	0.327	
⁹¹ Kr	3.267	0.100	3.049	0.324	
⁹² Rb	3.110	0.086	2.471	0.158	
⁹⁷ Y	3.048	0.110	3.265	0.218	
sum	38.237		38.342		

Table I: Comparison of fission yields data at 0.0253 eV of ²³⁵U with experimental data for 10 nuclides

W. Lang measured fission product yields of which masses range from 80 to 107. Most abundant 10 nuclides among them are compared with the result of GEF code in table I. The mass distributions show good agreements and yield of each nuclide doesn't show big difference. The measurements and calculated results of the fission yields should be carefully compared considering normalization methods, experimental conditions, uncertainties, etc. for one to one comparison. Especially, normalization for comparison should be carefully performed because the number of fission products from experiments and GEF simulation is not same.

3.3 Comparison with existing nuclear data libraries

GEF code generates independent fission yields of the fission fragments according to atomic number, neutron number, mass number and isotopes, respectively. Yields sum of fission products is normalized to 200. Comparing with yields data of recent nuclear data libraries such as ENDF/B-VII.1, JEFF-3.1.1 and JENDL/FPY-2011, GEF provides relatively narrow ranges of nuclides. Table II shows the range according to nuclides, mass numbers and atomic numbers of fission products generated from 235 U thermal fission process. GEF code gives fission product yields of which mass numbers lie from 73 to 162 while the mass number ranges of those are from approximately 65~170 in available nuclear data libraries. The number of nuclides produced from fission process is more than 2 times. This doesn't mean that the results of GEF code are not comparable with the libraries.

Table II: Comparison of fission products produced from ²³⁵U thermal fission

	ENDF/B- VII.1	JEFF- 3.1.1	JENDL/ FPY-2011	GEF code
No. of Nuclides	998	919	1067	437
Range of Mass	107	119	116	89
Range of Atomic No.	47	50	52	35

The most plentiful 10 nuclides, which are produced from ²³⁵U fission process induced by thermal neutron, are listed in table III in order of large yields. Although the order is slightly different, the contents of top10 nuclides are almost same. In spite of a small number of fission products, the results of GEF code cover most of important nuclides produced by nuclear fission process. The yields sum of most abundant 437 fission products reaches at 99.995%, 99.993% and 99.993% of ENDF/B-VII.1, JEFF-3.1.1 and JENDL/FPY-2011 yield sum, respectively.

Table III: Comparison of ²³⁵U 10 abundant fission yields data at 0.0253 eV of ENDF/B-VII.1, JEFF-3.1.1 and JENDL/FPY-2011

ENDF/	F/B- JEFF-3.1.1		JENDL/FPY-		GEF code		
VII.1				2011			
nuclide	yield	nuclide	yield	nuclide	yield	nuclide	yield
¹³⁴ Te	6.22	¹³⁴ Te	6.00	¹³⁴ Te	6.21	¹³⁴ Te	6.30
¹⁰⁰ Zr	4.98	¹³⁸ Xe	4.95	¹⁰⁰ Zr	4.97	¹³⁸ Xe	5.48
¹³⁸ Xe	4.81	¹⁰⁰ Zr	4.90	¹³⁸ Xe	4.81	⁹⁴ Sr	5.14
⁹⁵ Sr	4.54	⁹⁴ Sr	4.70	⁹⁵ Sr	4.53	⁹⁵ Sr	4.81
⁹⁴ Sr	4.51	⁹⁵ Sr	4.67	⁹⁴ Sr	4.51	¹³⁹ Xe	4.47
⁹⁰ Kr	4.40	¹³⁹ Xe	4.57	⁹⁰ Kr	4.39	100 Zr	4.41
¹³⁹ Xe	4.32	⁹⁰ Kr	4.50	¹³⁹ Xe	4.32	⁹⁶ Sr	4.25
¹⁴³ Ba	4.10	¹⁴⁴ Ba	4.21	¹⁴³ Ba	4.10	⁹⁰ Kr	3.96
¹⁴⁴ Ba	3.97	99Zr	3.99	¹⁴⁴ Ba	3.97	99Zr	3.95
⁹⁹ Zr	3.58	¹⁴³ Ba	3.98	⁹⁹ Zr	3.58	¹⁴⁴ Ba	3.93

sum	45.4	sum	46.5	sum	45.4	sum	46.7
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Fig. 4. Comparison of fission product yields with mass in ENDF and JEFF with GEF results for ²³⁵U thermal fission. Except light nuclides less than mass number 20, overall shape is well reproduced by GEF code.

Figure 4 shows fission product yields with mass in ENDF/B-VII.1 and JEFF-3.1.1 and GEF results for 235 U thermal fission. GEF produces general trend of fission product mass distribution quite well. The right parts of figure 4 in blue circle are light fission products of which mass numbers range from 1~21. GEF, like other nuclear reaction calculation programs such as TALYS, does not consider the production of light nuclide.



Fig. 5. 235 U fission product yields with mass by GEF were compared with ENDF/B-VII.1 at 500 keV and 14 MeV.

Figure 5 shows ²³⁵U fission product yields with mass at 500 keV and 14 MeV, respectively. Even though there are large differences for low yield nuclides, GEF code anticipates general trend of mass distribution of fission products so well.

4. Conclusion and Future Work

The GEF code is very powerful tool to generate fission yields without measurements. Also, it can produce the distribution of fission product yields for continuous neutron energy while measured data are given only at several energies.

The fission yields data of ²³⁵U have been tentatively generated with GEF code in this work. Comparing GEF results with measurements and recently released evaluated fission yields data, it is confirmed that GEF code can successfully predict the fission yields data. With its sophisticated model, GEF code is playing a significant role in nuclear industry.

Our future work will be a domestic database production of fission yields data with GEF and measured data. And then the fission yields database will be validated through the benchmark tests.

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