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Prompt and Delayed Neutron Emissions and Fission Product Yield Calculations with Hauser-Feshbach Statistical Decay Theory and Summation Calculation Method

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Abstract. We demonstrate the neutron emission and fission product yield calculations using the Hauser–Feshbach Fission Fragment Decay (HF^{3}D) model and β decay. The HF^{3}D model calculates the statistical decay of more than 500 primary fission fragment pairs formed by the neutron induced fission of ^{235}U. In order to calculate the prompt neutron and photon emissions, the primary fission fragment distributions, i.e. mass, charge, excitation energy, spin and parity are deterministically generated and numerically integrated for all fission fragments. The calculated prompt neutron multiplicities, independent fission product yield are fully consistent each other. We combine the β-decay and the summation calculations with the HF^{3}D model calculation to obtain the cumulative fission product yield, decay heat and delayed neutron yield. The calculated fission observables are compared with available experimental data.

1 Introduction

The nuclear data of fission yields are essential ingredients for numerous nuclear applications such as the conception of new generation of reactors and nuclear fuel cycle developments. With increase in requirements by those applications, fission yields from wide variety of actinides and wide ranges of energy have become of great interest.

Numerous theoretical efforts have been made with both microscopic and macroscopic methods to understand the fission dynamics. These approaches provide a quantum description of the fission dynamics and mass, kinetic energy distributions of excited fission fragments. Dynamical description of fission by Langevin equations is one of the examples, which can treat the deformation of each fragment independently and allows us to analyse key information about fission fragments such as mass distribution and total kinetic energy (TKE) [1].

These fission fragments formed just after fission will evaporate prompt neutrons and photons to reach their ground state or meta-stable state. Many models and codes have been developed for the study of prompt neutron and photon emissions, and yield distribution to reproduce experimental results. One of the reliable approaches is the Hauser-Feshbach stastical decay of fission fragments.

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The post-neutron emitted fission fragments, so called fission products, will β decay that leads the β-delayed neutron and photon emissions, to reach the stable isotopes. Many efforts have been done to understand beta decay properties of nuclei far away from beta stability. Theoretical approach such as the gross theory treats the sum of strengths of the transition from initial to final states in quantum mechanics [2]. For reactor application purpose, summation calculation has been used for the prediction of the decay heat from fission products. The summation calculation requires information about half-lives, γ- and β-energies released in the decay. Since the decay can proceed via a very large number of excited levels, the decay data have been evaluated and provided as an evaluated library such as ENDF/B-VII.1 decay data library.

However, an accurate prediction of fission observable through out the fission (pre prompt emissions), de-excite and the beta decay processes by theoretical calculations in a consistent manner still remains difficult. Therefore the evaluations of nuclear data have been done inconsistently [3] and some ingredients have been provided based on some empirical models.

We demonstrate the calculations of the fission observables such as independent/cumulative fission product yields (FPY), prompt/delayed neutron and photon emissions, and decay heats in a consistent manner starting from a unique fission fragment distribution until all fission fragment pairs de-excite and β decay until they reach to their stable isotopes. We employ the Hauser-Feshbach Fission Fragment Decay (HF^{3}D) model to calculate the prompt neutron multiplicity and the independent FPY [4]. The β-decay chains of each nuclide in the independent FPY are tracked to obtain the cumulative FPY by using ENDF/B-VII.1 decay data library. The decay heat and delayed neutron yield are calculated by the summation calculation method using a Oyak computer code [5] that also incorporates ENDF/B-VII.1 decay data library. The calculated results are compared with experimental data and the evaluated nuclear data libraries.

2 Method

For the de-excitation process of the fission fragments, we employed the HF^{3}D model [4]. The main features of the HF^{3}D model are (1) generation of the distributions of mass and charge yields, excitation energy, level density, spin, and parity $Y(A, Z, E_{ex}, J, \Pi)$ for all primary fission fragments, and (2) integration over all these distributions. More than 500 fission fragment pairs are generated by the HF^{3}D model for ^{235}U. The concept of the generation of the fission fragment distributions by the HF^{3}D model is discussed in Ref [4]. The mass distribution of primary fission fragment yield $Y(A)$ is generated from the five Gaussians fitted to the experimental data. The charge distributions of every mass number are generated using the Wahl systematics (Z_P model) [6] to fill the fission fragment distribution. The experimentally available total kinetic energy TKE(A) distribution is fitted by analytical functions in order to generate total excitation energy (TXE) distributions for fragment pairs. The TXE can be calculated from TKE by taking into account the energy balance of the reaction. The HF^{3}D model calculates the neutron multiplicities $\overline{\nu}^{(k)}_{l,h}$ for the k-th pair of fission fragments by integrating the neutron evaporation spectrum $\phi^{(k)}_{l,h}$ from the light or heavy fragment in the center-of-mass system,

$$\overline{\nu}^{(k)}_{l,h} = \int dE_x \sum_{J\Pi} \int d\epsilon\, R(J,\Pi) G(E_x) \phi^{(k)}_{l,h}(J,\Pi,E_x,\epsilon)\,, \tag{1}$$

where $R(J,\Pi)$ is the probability of nucleus having the state of spin J and parity Π, and $G(E_x)$ is the distribution of excitation energy. By performing this calculation for each fission fragment pair, one can obtain the prompt neutron spectrum $\chi(E)$ and multiplicities $\overline{\nu}$, and the independent FPY $Y_I(A,Z)$ from ^{235}U(n,f).

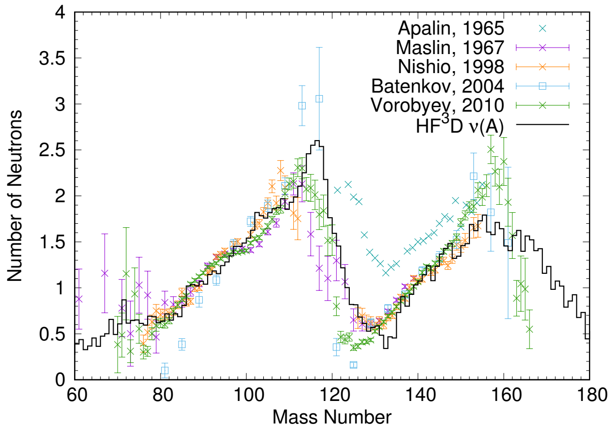

Figure 1. The mass dependent neutron multiplicity for ^{235}U(n_{th},f) calculated with the HF^{3}D model compared with experimental data.

For the Hauser-Feshbach calculations, the neutron optical potential by Koning-Delaroche, level density systematics based on the KTUY05 mass model, and the Kopecky and Uhl γ-ray strength function for the E1 transition, and the standard Lorentzian model for higher multipolarities are used.

For the β-decay process, the cumulative FPY was obtained by performing the β-decay calculation of the nuclides for the calculated independent FPY by tracing the β-decay path using the ENDF/B-VII.1 decay data library. The β- and γ-energy components in the decay heats, and delayed neutron yield were calculated by the summation calculations method [5].

3 Results and Discussion

3.1 Prompt neutron multiplicity

The calculated average neutron multiplicity $\overline{\nu}$ for ^{235}U(n_{th},f) was 2.38 which is 2.5% smaller than the evaluated value in JENDL-4.0 ($\overline{\nu}$ = 2.44). The mass dependent neutron multiplicity $\overline{\nu}(A)$ is shown in Figure 1 together with available experimental data [7–11]. Our calculation well follows the experimental data in the range with the mass number 60<A<150. Generally, simulations rarely calculate $\overline{\nu}$ for mass ranges A<60 and 150<A when the Monte Carlo technique is used for generations of fission fragment distributions because the fission fragment yields are too small to sample in these ranges, whilst our calculation gives $\overline{\nu}$. This is because our calculation is based on the deterministic method. However, such small yields in this mass range also makes experiment difficult and as a concequence experimental data has a large uncertainty.

3.2 Fission product yield

Figure 2 illustrates the mass dependence of the independent FPY for ^{235}U(n_{th},f). Our calculation well reproduces the distribution of independent FPY in JENDL/FPY-2011 for small peaks at A = 99 and 134, and the tendency of independent FPY in the wide range of mass numbers which varies from 10^{-11} to 10^{-2}.

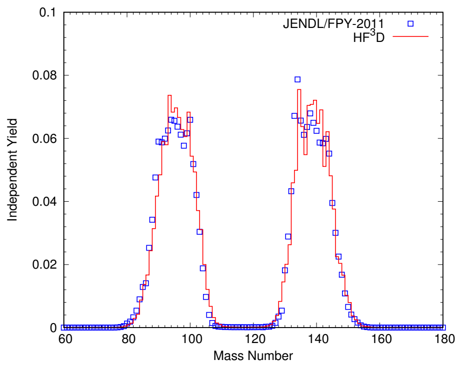

Figure 2. The mass total independent FPY of ^{235}U(n_{th},f) calculated by the HF^{3}D model and the evaluated data in JENDL/FPY-2011

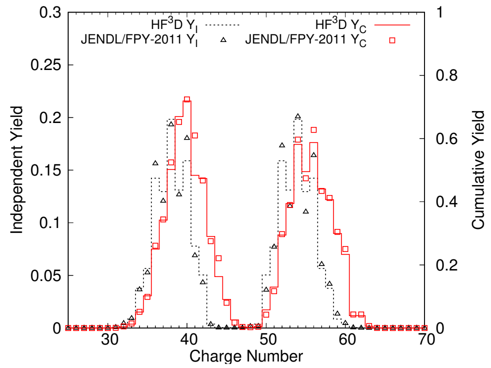

Figure 3. The charge total independent and cumulative FPY of ^{235}U(n_{th},f) calculated by the HF^{3}D model and the evaluated data in JENDL/FPY-2011.

The cumulative FPY was obtained by performing the β-decay calculation using the calculated independent FPY. Since the post-neutron emitted (independent) fission product decays by β-decay path in the same mass number and β-delayed neutron emission yield is quite small to give an obvious change in the mass dependent fission yield, we compare the charge dependent fission yield before and after the β-decay. Figure 3 shows the charge dependence of the independent and cumulative FPYs for ^{235}U(n_{th},f). The calculated cumulative FPY well reproduces the evaluated data in JENDL/FPY-2011. By comparison between the independent and cumulative FPYs, the β-decay calculation successfully tracks the β-decay chains for each nuclide in the independent FPY data and reproduces the cumulative FPY.

3.3 Summation calculations

We have performed a set of preliminary calculations of the summation method. The calculated decay heats by β and γ emissions are shown in Figure 4 together with the experimental data of Lowell and Oak Ridge National Laboratory for ^{235}U(n_{th},f). The major differences in the decay heat from the γ emissions below 10 second after the fission burst is mainly due to an over-estimation of the independent FPY of ^{97g}Y and some other nuclides. In addition, the calculation strongly depend both on the independent FPY and the decay data library that is used to track the β-decay chain and sum-up the energy release from both the β and γ emissions.

The calculated total average number of delayed neutrons per fission ($\overline{\nu}_d$) for ^{235}U(n_{th},f) is 0.01659. The calculated result is 4.7% higher than evaluated value in JENDL-4.0 ($\overline{\nu}_d$=0.01585). Figure 5 shows the cooling time dependence of calculated $\overline{\nu}_d$ compared with the experimental data. There are some nuclides that are over-estimated in the independent FPY, e.g. ^{94,95}Rb and ^{96}Y, compared to the evaluated nuclear data libraries. These nuclides strongly affect $\overline{\nu}_d$.

It is worth mentioning that we did not introduce any adjustments at each calculation step in this study. In order to reproduce experimental data more accurately, one can optimize the starting distributions and can introduce some constrains. The deterministic method to generate the distributions loses correlation information among the distributions. However, this method is quite effective to examine the fission fragment distributions which are generated by the theoretical simulation of fission process such as the Langevin method, because many of comparable fission observables are after the β decay. Such the connection also makes pos-

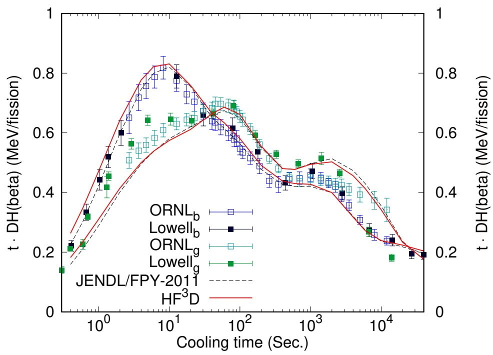

Figure 4. Cooling time dependence of the decay heats by β (b) and γ (g) emissions comparing with the experimental data for ^{235}U(n_{th},f).

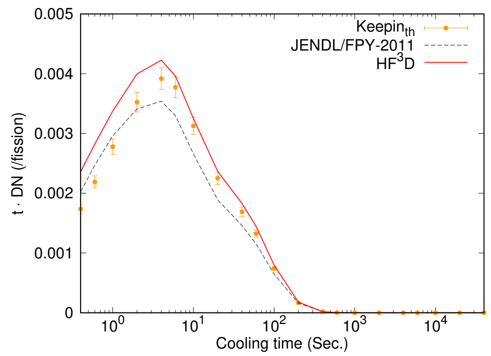

Figure 5. Cooling time dependence of the delayed neutron yield comparing with the experimental data for ^{235}U(n_{th},f).

sible to expand the nuclear data evaluation for variety of actinides and wide range of incident neutron energies.

4 Conclusion

In this work we demonstrated a fully consistent approach to calculate some fission observables starting from a unique fission fragment distribution. We employed the recently developed Hauser-Feshbach fragment decay model, HF^{3}D, to calculate the prompt neutron multiplicity and the independent FPY. The β-decay path of each fission product is tracked using the ENDF/B-VII.1 decay data library to obtain the cumulative FPY. The decay heat and delayed neutron yield are calculated by the summation calculation method. All obtained fission observables were compared with the experimental data and showed fairly good agreement with experimental tendency without any parameter adjustments. The scalability of the combination of HF^{3}D model, β-decay, and summation calculation enables us to perform series of consistent calculations for the other actinides and energy ranges. We have performed a set of preliminary calculations of the incident energy dependent prompt and delayed neutron emissions [12].

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