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Implementation of the Hauser-Feshbach theory for Fission Product Yield Evaluation and Fission Modelling

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The IAEA-NDS would appreciate any comment on this report at: nds.contact-point@iaea.org.

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Abstract

The special meeting focused on the Implementation of the Hauser-Feshbach theory for Fission Product Yield (FPY) Evaluation and Fission Modelling was held at IAEA Headquarters in Vienna from 13 to 17, January 2020, as a joint effort among JAEA, LANL and IAEA Nuclear Data Section. The meeting was a preparatory work toward new FPY data libraries planned at each institute. We discussed implementation of the Hauser-Feshbach statistical decay model to calculate the de-excitation of fission fragments, and performed inter-comparison of the available three codes at each institute — CCONE (JAEA), CoH/BeoH (LANL), and TALYS (IAEA). The discussions include types of fission observable to which we can produce by our models, estimation of initial fragment configurations (after scission and before prompt particle emission), and future development of these codes to make them applicable for the FPY data evaluation.

Table of contents

1	Introduction	5
2	Procedures	7
2.1	The Hauser-Feshbach modelling	7
2.2	Calculated quantities that can be compared with experimental data	8
3	Fission fragment distributions	9
3.1	Fission fragment distribution model	9
3.2	Generation of the primary fission fragment yield	9
4	Inter-comparison of the Hauser-Feshbach codes	12
4.1	Simple Hauser-Feshbach decay comparisons for ^{139}Xe	12
4.2	Decay from specific initial excitation energy and spin/parity distributions .	12
4.3	Prompt neutron multiplicity from simple fragment pairs decay calculation .	13
4.4	Future work	14
5	Summary	15

1 Introduction

The meeting on the "Implementation of the Hauser-Feshbach theory for Fission Product Yield Evaluation and Fission Modelling" was held at the IAEA Headquarters, Vienna, Austria from 13th to 17th of January 2020, aiming to exchange expertise of fission modeling and to enhance model code capabilities at Japan Atomic Energy Agency (JAEA), Los Alamos National Laboratory (LANL) and IAEA Nuclear Data Section toward new Fission Product Yield (FPY) data evaluations at each institute. We discussed a method to utilize the Hauser-Feshbach statistical decay theory [1] in the de-excitation process of fission fragment pairs produced just after scission. Currently there exist at least three codes that include the Hauser-Feshbach decay model for FPY — CCONE (Version:0.9.4.9.1) [2, 3] at JAEA, CoH/BeoH[4, 5] at LANL, and TALYS [6] at IAEA NDS. In this study, inter-comparison of these codes by performing some simple calculations identified several issues to be considered in order to apply the Hauser-Feshbach model codes to the FPY data evaluations.

The FPY is one of the key ingredients in many nuclear energy application fields. Thanks to recent advances in theoretical models and computational infrastructure, we are able to estimate various properties of fission fragment at scission nowadays. However, our current knowledge of nuclear fission theory is not yet at the level of producing the FPY that are accurate enough for practical applications.

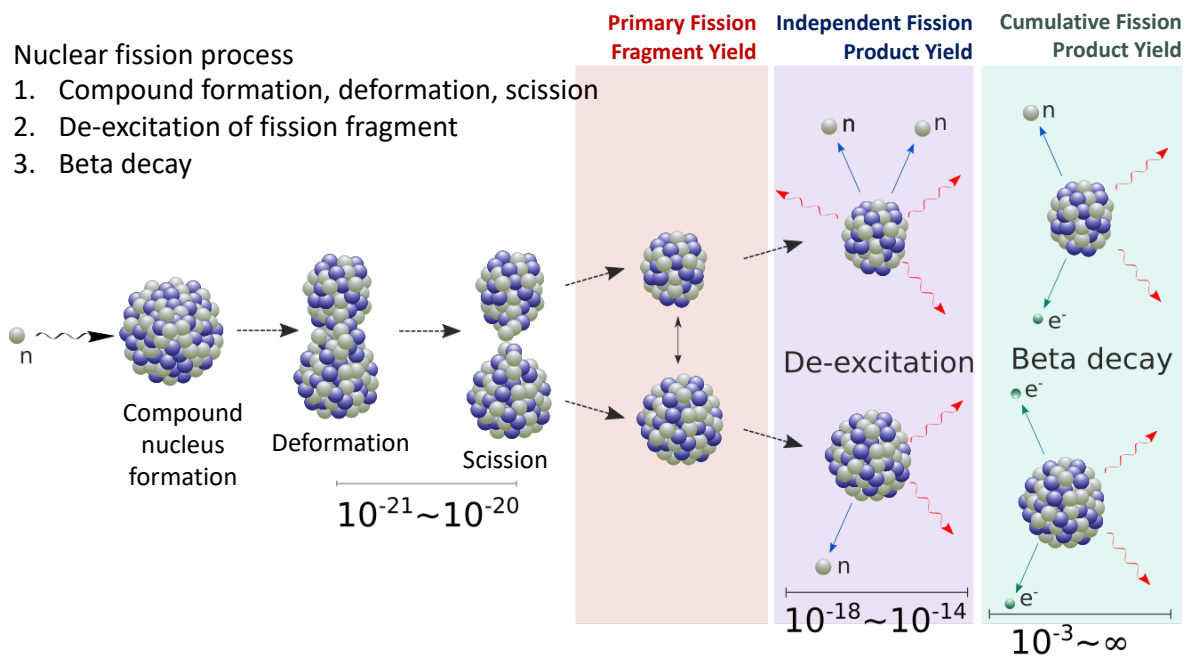


Figure 1: Schematic view of the nuclear fission.

Figure 1 shows the schematic view of the time evolution of nuclear fission process. In the case of neutron-induced fission on an actinide, a dynamical process of nuclear fission is initiated by formation of a compound nucleus, then large amplitudes of collective motion leads to scission of the compound nucleus. The nuclear fission produces two highly excited fragments, which decay by emitting several prompt neutrons and γ -rays. We interpret this de-excitation process by the Hauser-Feshbach statistical decay theory. A set of distributions that characterize the primary fission fragment yield $Y(Z, A, E_{EX}, J, \pi)$, such as mass A , charge Z , excitation energy E_x , spin J , and parity π , is the principal input of the Hauser-Feshbach statistical decay calculation. We test the sensitivity of the given fission fragment yields to the prompt fission observable

for the particularly important reaction $^{235}\text{U}(\text{n}_{\text{th}},\text{f})$, where experimental data are relatively abundant.

The statistical decay of fission fragments generates the independent FPY, $Y_I(Z, A, M)$, where M stands for the meta-state flag. The cumulative FPY $Y_C(Z, A, M)$ and β decay observables such as the delayed neutron yield ν_d are given by solving the Bateman equation in a time-dependent manner, or can be directly calculated as $dY/dt = 0$. For example, time evolution of the delayed neutron $\nu_d(t)$ requires the Bateman equation, while the average number of delayed neutrons $\bar{\nu}_d$ does not. Anyway, in both cases the nuclear decay data library plays an essential role. Experimental data of $Y_C(Z, A, M)$ and other relevant quantities also determine the parameters in the statistical decay model retroactively.

Eventually one needs to have a precise parameterization of the initial distributions to be used as inputs of the Hauser-Feshbach calculation from an analysis of experimental data. In this scope, it is important to have the same experimental FPY dataset as a common basis of new parameterizations. Therefore, we also review some available experimental data for $^{235}\text{U}(\text{n}_{\text{th}},\text{f})$ as an example.

This report summarizes discussions on applying the Hauser-Feshbach decay model to the FPY calculation. We perform inter-comparison of the existing model codes, CoH/BeoH, CCONE, and TALYS, which are already capable for calculating FPY with the Hauser-Feshbach theory. Although the β -decay of the produced fission products was discussed in this meeting with a specialist at IAEA NDS [7], we decided to study these topics separately, and briefly mentioned two recent papers of Kawano and Chadwick [8], and Minato [9].

2 Procedures

2.1 The Hauser-Feshbach modelling

We employ the Hauser-Feshbach statistical decay theory [1] for the fragment de-excitation process. The probabilities of neutron and γ -ray emissions from a compound state are calculated with neutron and γ -ray transmission coefficients, where the particle and photon competition is always included at each stage of compound state decay, as shown in Fig. 2.

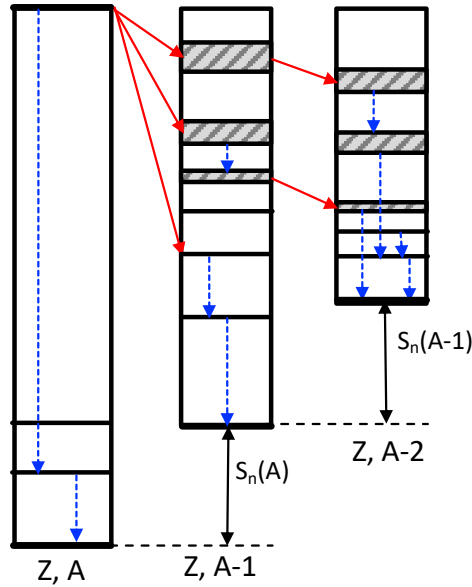


Figure 2: Schematic view of the multiple neutron and γ -ray emission process from a compound nucleus, (Z, A) . The solid arrows represents the neutron emission, and the dotted arrows represents the γ -ray emission.

To perform the Hauser-Feshbach statistical decay calculation, we need to characterize an initial configuration of fission fragments, namely the excitation energy, spin and parity distributions, as well as a combined distributions $Y(Z, A, \text{TKE})$ of fragment mass A , charge Z , and total kinetic energy TKE. These distributions are often obtained by some theoretical and/or phenomenological models for the dynamical fission process. For the neutron-induced fission case, the total excitation energy TXE can be calculated by the energy conservation

$$\begin{aligned}
 \text{TXE}(Z_l, A_l, Z_h, A_h) &= Q - E_{inc} - \text{TKE}(Z_l, A_l, Z_h, A_h) \\
 &= E_{inc} + B_n(Z_c, A_c) \\
 &+ [M_n(0, 1) + M_n(Z_c, A_c) - M_n(Z_l, A_l) \\
 &- M_n(Z_h, A_h)] - \text{TKE}(Z_l, A_l, Z_h, A_h), \quad (1)
 \end{aligned}$$

where the suffixes l, h and c denote the light, heavy fragments and fissioning compound nucleus, Q is the reaction Q -value for this particular separation, and M_n represents the nuclear mass in the unit of energy.

TXE is divided into two fragments, $\text{TXE} = E_l + E_h$, and each fragment will have the excitation energy that might be roughly proportional to the available number of states, so that a naive ansatz could be

$$\int_0^{E_l} \rho_l(E_x) dE_x \simeq \int_0^{E_h} \rho_h(E_x) dE_x, \quad (2)$$

and considering the level density of light fragment ρ_l is lower than ρ_h , $E_l > E_h$. When the level density parameter a is proportional to the mass A , the excitation energy ratio reads $E_l/E_h = A_h/A_l$, which is temporarily adopted by CCONE. Ohsawa et al. [10] proposed a method to split TXE into the pair of fission fragments by considering the ratio of nuclear temperature, and the same technique is employed by different fission modelings [11, 12, 13, 14, 5, 15]. The ratio of nuclear temperature is expressed by the anisothermal parameter R_T as

$$R_T = \frac{T_l}{T_h} = \sqrt{\frac{U_l a_h(U_h)}{U_h a_l(U_l)}}, \quad (3)$$

where $a(U)$ is the shell-effect corrected level density parameter at the excitation energy U . Re-distributing TKE into two fragments changes many fission observables, particularly the prompt neutron multiplicity $\bar{\nu}_p$. Since TKE in Eq. (1) has some distribution, the obtained E_l and E_h also have corresponding widths [5].

The spin J and parity Π distribution is often assumed to be a Gaussian form

$$R(J, \Pi) = \frac{J + 1/2}{2f^2\sigma^2(U)} \exp\left\{-\frac{(J + 1/2)^2}{2f^2\sigma^2(U)}\right\}, \quad (4)$$

where $\sigma^2(U)$ is the spin cut-off parameter in a level density model, and f is a scaling factor [5]. Instead of scaling the spin-cutoff factor in the level density model, Becker et al. [11] directly models the spin-cutoff factor B^2 .

An optical potential for neutron, γ -ray strength functions, and nuclear level densities are also essential ingredients for such decay calculations. However we do not explore impact of these parameters in this report.

2.2 Calculated quantities that can be compared with experimental data

The results of statistical decay calculations may be post-processed to construct some fission quantities, which are then compared with available experimental data. Typical quantities that are often given in literature are summarized in Table 1. Although this is a wish list, we compared $\bar{\nu}$ only during the meeting. We do not compare all of the quantities, since these output options in many of the Hauser-Feshbach codes are not yet operational.

Table 1: Representative fission quantities comparable to experimental data.

Type	Description
$Y_i(A)$	Independent fission yield as a function of mass number
$Y_i(Z, A, M)$	Independent fission yield of all isotopes including meta-stable state
$\bar{\nu}$	Average number of neutrons per fission
$\bar{\gamma}$	Average number of γ -rays per fission
$\bar{\nu}(A)$	Average neutron multiplicity as a function of fission product mass
$\bar{\gamma}(A)$	Average γ -ray multiplicity as a function of fission product mass
$\langle E_n \rangle$	Average prompt neutron energy
$\langle E_\gamma \rangle$	Average prompt γ -ray energy
$\langle E_n \rangle(A)$	Average neutron energy as a function of product mass
$\langle E_\gamma \rangle(A)$	Average γ -ray energy as a function of product mass
$P(\nu)$	Neutron multiplicity distribution
$\chi(\nu)$	Prompt fission neutron energy spectrum (PFNS)
$\phi(\gamma)$	γ -ray energy spectrum

3 Fission fragment distributions

3.1 Fission fragment distribution model

Table 2 shows a list of typical experimental data, which are required to generate distributions of the fission fragment before neutron and γ -ray evaporation calculations are performed.

Table 2: Experimental data used for fitting of primary fission fragment distributions

Type	Descriptions
$Y_{pre}(A)$	Primary (Pre-neutron emission) fission fragment mass distribution
$Y_{pre}(Z, A)$	Primary (Pre-neutron emission) fission fragment mass and charge distribution
TKE(A)	Total kinetic energy of fission fragments as a function of primary fission fragment mass
σ TKE(A)	The width of total kinetic energy of primary fission fragments

An empirical systematics of FPY proposed by Wahl [16], known as Wahl systematics, generates the independent FPY $Y_I(Z, A)$. The primary fission fragment mass distributions $Y(A)$ in the Wahl systematics are expressed by 3 to 5-Gaussian functions. The isobaric charge distribution is generated by the Z_p model [17]. The Gaussian centroid, width, and fractions, together with all other model parameters involved, were determined by the least square fitting to available experimental data. The prompt neutron multiplicity is also estimated and modeled by looking at experimental $\bar{\nu}(A)$ data and subtracted $\bar{\nu}(A)$ from $Y(A)$. ENDF FPY data evaluation [18] largely employed the Wahl systematics.

Similar to the Wahl systematics, Katakura also parameterized the FPY by applying the 5-Gaussian function [19], but he directed his model toward the energy variation of FPY, namely from thermal to high energy fission reactions. The Gaussian parameters are determined mainly by the experimental data of Zöller et al. [20] and Dickens [21], while $\bar{\nu}(A)$ is the same Wahl systematics. Since the isobaric charge distribution is not defined in the Katakura systematics, one has to model it somehow. In the current modeling in CCONE combines $Y_I(A)$ by the Katakura systematics and a simple Gaussian for the Z -distribution, where the most probable Z is calculated as $Z_{UCD} \pm 0.5$ for the light and heavy fragments, and their fixed width 0.493 was determined empirically. Z_{UCD} is the peak-location of the so-called unchanged charge distribution.

3.2 Generation of the primary fission fragment yield

The three codes use different fission fragment yield distribution; CoH/BeoH has the 5-Gaussian functions determined from available experimental data [5], CCONE implants Katakura's systematics that comprise 5-Gaussian functions [19], TALYS invokes the GEF code [22] to generate $Y(Z, A)$ as well as the mean excitation energy \bar{E}_{ex} and its width. The exact parameterization employed in TALYS/GEF was not so clear yet, although we investigated the code output during the meeting.

Figures 3 and 4 show the experimental fission fragment yields and TKE as a function of fragment mass adopted in CoH/BeoH [5]. The isobaric charge distributions are generated from Z_p model implemented in CoH/BeoH. TKE is then converted into TXE by Eq. (1), and divided into E_l and E_h by Eq. (3). See Ref. [5] more in detail.

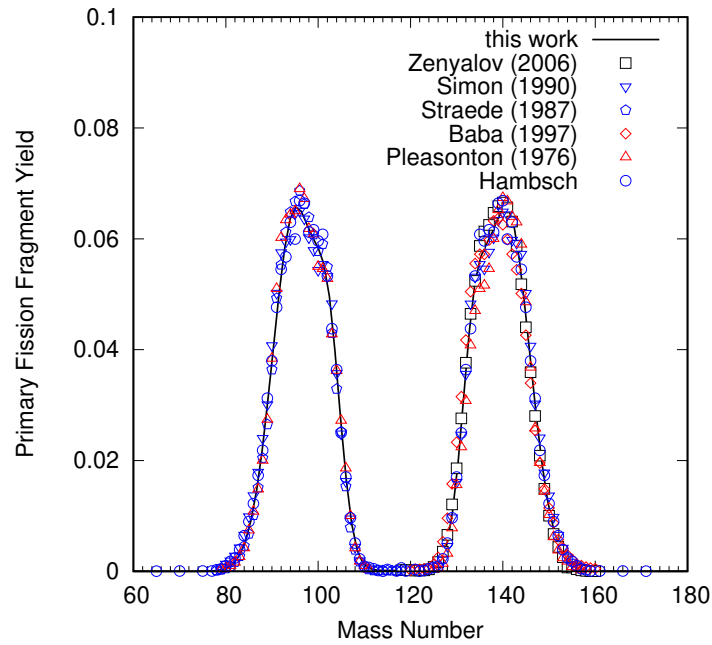


Figure 3: Pre-neutron emission mass yield by fitting to the experimental data using 5 Gaussian functions.

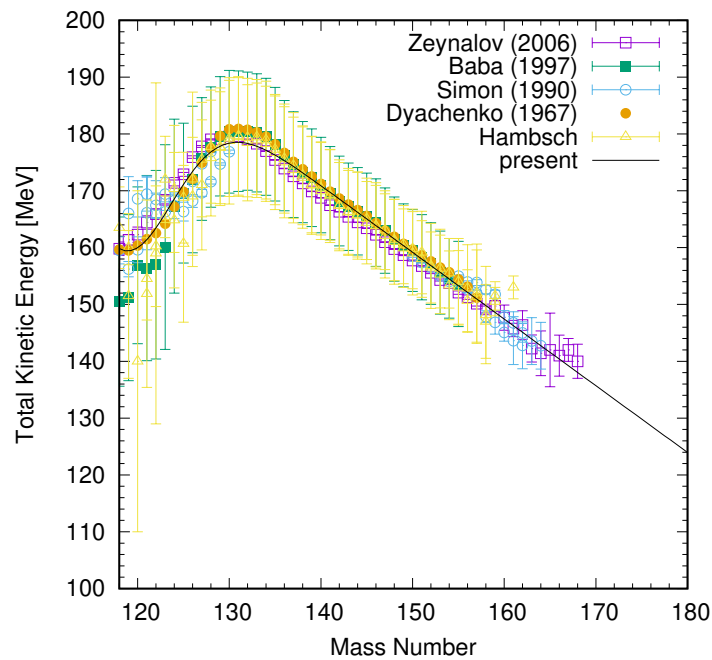


Figure 4: Experimental total kinetic energy as a function of fragment mass together with fitted line.

Figure 5 shows $Y(A)$ of the Katakura systematics [19] for the thermal neutron induced fission on ^{235}U case, which was implemented in CCONE. Katakura's systematics somehow disagrees with the experimental trend in this case, especially at the peak locations, because the analysis didn't put heavy weight on this particular energy point.

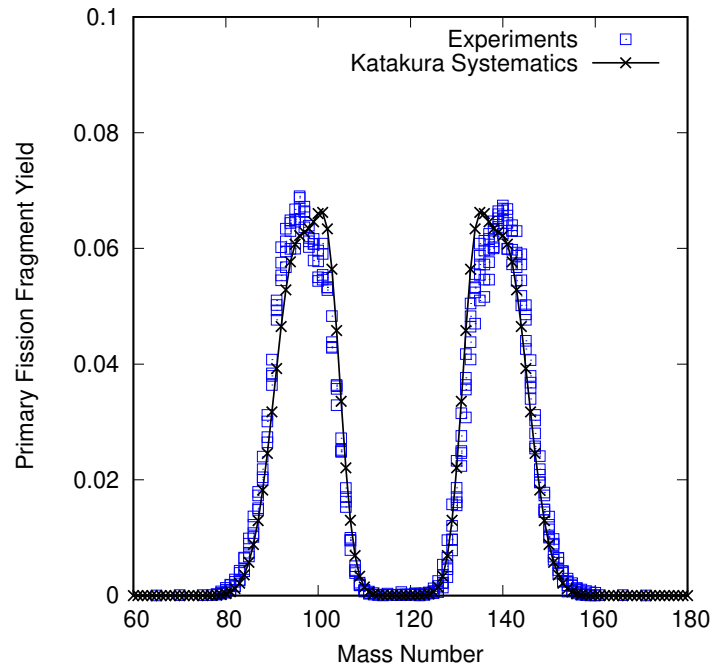


Figure 5: Pre-neutron emission mass yield together with fitting lines generated in CCONE code with 5 Gaussian functions model developed by Katakura [19].

Figure 6 shows $Y(A)$ of the thermal neutron induced fission of ^{235}U , which is implemented in TALYS (a version currently under development). In this study, TALYS implements the same $Y(A, Z)$ and a similar excitation energy distribution for each fission fragment pairs as in CoH/BeoH for a test case.

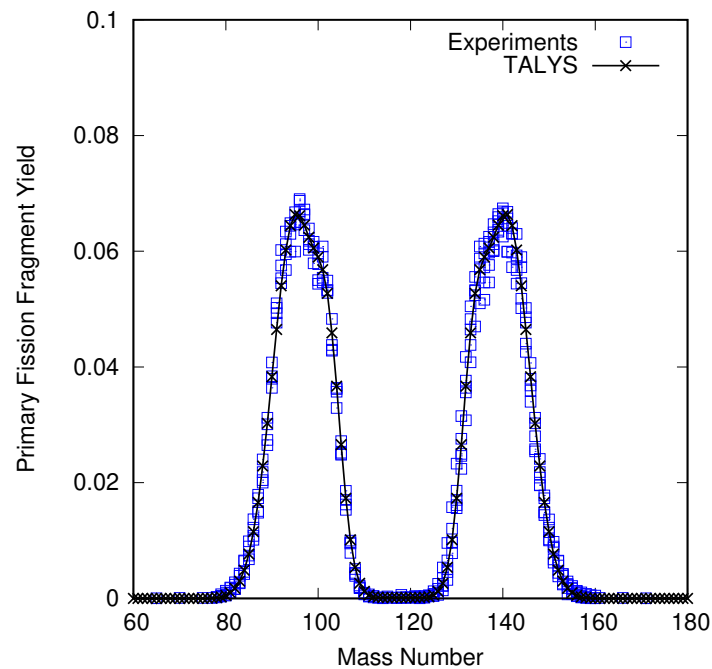


Figure 6: Pre-neutron emission mass yield implemented in TALYS (a version under development).

4 Inter-comparison of the Hauser-Feshbach codes

As a preparatory study on the Hauser-Feshbach decay for fission fragments, we conducted two numerical calculations and compare our current modeling in CoH/BeoH, CCONE, and TALYS. This exercise was aiming at minimizing the influence of model implementation, and see if we will be able to obtain a consistent result when the same model parameters are provided.

4.1 Simple Hauser-Feshbach decay comparisons for ^{139}Xe

The first test is a simple Hauser-Feshbach decay calculation from an artificially formed compound state in ^{139}Xe , at 15 MeV excitation and $J^\pi = 2^+$. This can be performed by filling that energy bin by a unit initial population in the Hauser-Feshbach code, and let the system decay. The statistical decay results by these three codes are shown in Fig. 7. The calculated production probabilities of the decay products $^{136-139}\text{Xe}$ agrees very well. Note that we didn't specify the model parameters in this test, so that each code runs by employing a default choice of the internal parameter set. Only a common choice is the neutron optical potential, which is the Koning-Delaroche [6]. Differences in the level density and the photon strength functions could have some impact in this comparison to some extent.

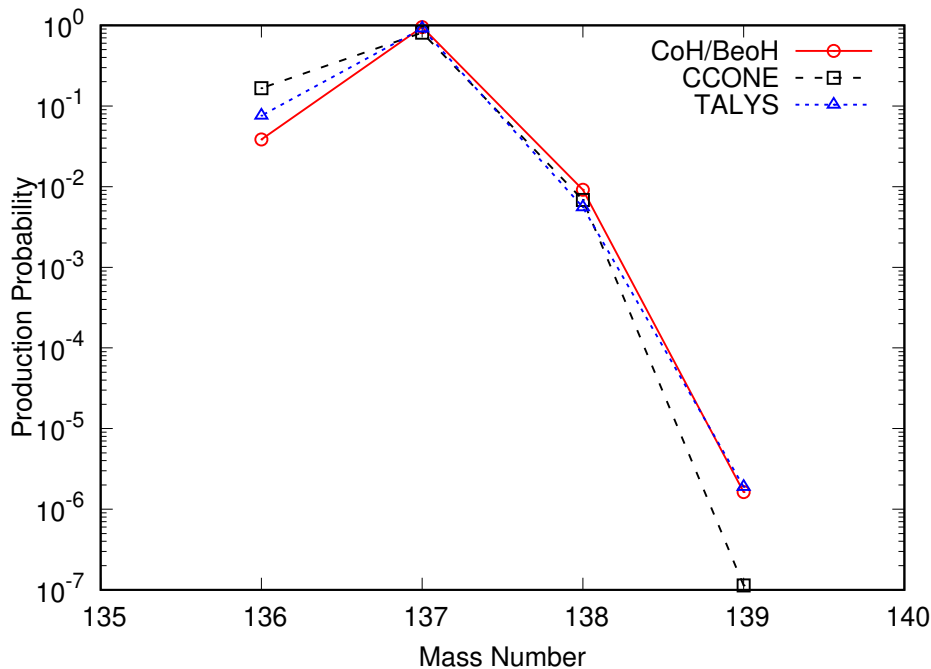


Figure 7: Production probability of residual nuclides from ^{139}Xe decay calculated from the simple condition. CoH/BeoH result is in open circle, CCONE result is in open square, and TALYS result is in open triangle.

4.2 Decay from specific initial excitation energy and spin/parity distributions

Next, we introduce an initial population distribution in ^{139}Xe as follows:

- In the excitation energy direction, we have a Gaussian distribution with the mean energy \overline{E} of 15 MeV and the width of 3 MeV;
- In the J (spin) direction, this is proportional to the spin distribution of the level density at a given excitation energy; and

- The highest energy, we take $\bar{E}(15 \text{ MeV}) + 2.5\sigma = 22.5 \text{ MeV}$.

Unfortunately CCONE was not able to control the mean excitation energy and width by an external input. We first ran CCONE and extracted the ^{139}Xe calculation part only, and found the internal values, which were $\bar{E} = 17.9 \text{ MeV}$ and the width of 5.95 MeV . Then we ran CoH/BeoH with this excitation energy distribution. As a result, this exercise was split into two cases; (A) the $\bar{E} = 15 \text{ MeV}$ case for CoH/BeoH and TALYS, and (B) the 17.9 MeV case for CoH/BeoH and CCONE.

The Hauser-Feshbach decay calculation begins at the top energy bin (at 22.5 MeV for case A and 17.9 MeV for case B), and continues all way down to the lowest energy bin or discrete level. This is equivalent to the integration over the excitation energy and spin distributions. The results are shown in Fig. 8. Since Case B has a higher total energy, the distribution of produced residuals shift toward the low-mass region (more prompt neutron emission). Some differences are seen in the no-neutron emission cases (production of ^{139}Xe). However, since they are really tiny probabilities and strongly depend on uncertainties in the photon strength function, this may not cause any large differences in a practical FPY evaluation.

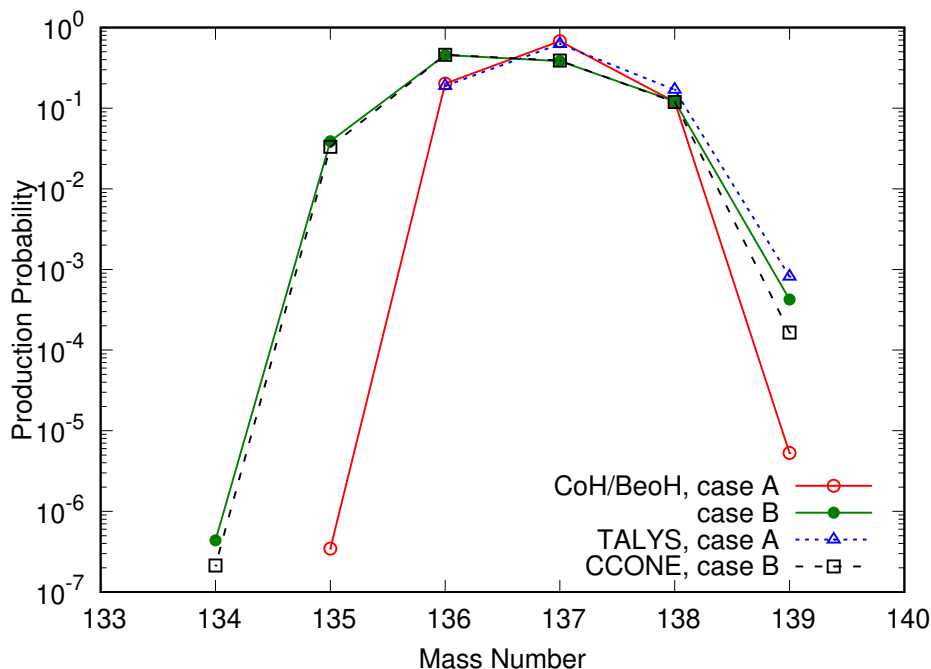


Figure 8: Production probability of residual nuclides from ^{139}Xe decay calculated from the simple condition. See Fig. 7 for legends.

4.3 Prompt neutron multiplicity from simple fragment pairs decay calculation

We briefly compared $\bar{\nu}$ calculated from fission fragment distributions that were generated from the systematics described in Section 3.2 with similar input conditions for CoH/BeoH and TALYS cases. Table 3 summarizes the calculated $\bar{\nu}$ together with the evaluated $\bar{\nu}$ in JENDL-4.0 and ENDF/B-VIII.0. Though preconditions are not entirely same, our results fairly agree with each other. Note that these values are preliminary results without any adjustments or optimizations.

Table 3: Preliminary results of calculated $\bar{\nu}$ from $^{235}\text{U}(\text{n},\text{f})$ at low energy (thermal or 1.0×10^{-6} MeV) together with evaluated data.

	$\bar{\nu}$
JENDL-4.0	2.43633
ENDF/B-VIII.0	2.42985
CoH/BeoH	2.45565
TALYS	2.40537 (at $E_{\text{in}}: 1.0 \times 10^{-6}$ MeV)

4.4 Future work

We summarize further works need to be implemented to the Hauser-Feshbach codes for the practical application of FPY data evaluations.

- Effects of multi-chance fission: Calculate systematically up to 5 MeV (approximate threshold energy of multi-chance fission) and combine 1-, 2-, n-chance fission contributions.
- β decay: Calculate β decay using $Y_I(Z, A, M)$ until all fission products reach to their stable isotopes $Y_C(Z, A, M)$, and calculate the decay heat and delayed neutron yield ν_d in a time dependent manner.
- Fission fragment modeling: Development of the formulations or systematics that are like Wahl systematics, which provide primary fission fragment distributions, principally for $Y(A)$ and $\text{TKE}(A)$, as a function of incident neutron energy.

5 Summary

The Hauser-Feshbach codes, CCONE [2, 3] at JAEA, CoH/BeoH[4, 5] at LANL, and TALYS [6] at IAEA NDS, which are capable for calculating de-excitation of fission fragments, were compared by paying a particular attention to a simple decay of fission fragment as a compound nucleus. In this meeting we shared information on implementation of the Hauser-Feshbach statistical decay model and necessary output quantities that can be compared with experimental data. We reported some results of the Hauser-Feshbach calculations using similar parameters of the primary fission fragment distributions as input, and discussed the differences among these codes. The results of simple decay calculations for a specific nuclide by these three codes exhibited relatively good agreement, while the entire set of fission fragment distributions $Y(Z, A, E_x, J, \pi)$ were found to be origin of the differences. Such distributions to be used as input of the Hauser-Feshbach calculations were briefly reviewed in order to establish a common basis of a new parameterization for future FPY evaluations. It should be noted that experimental primary fission fragment distribution data are always inferred from accessible post-prompt neutron/ γ -ray emissions and/or post- β decay distributions. Therefore, it is emphasized that development of empirical- or theoretical- model for the primary fission fragment distributions is equally important in the larger scope of FPY study.

Although our primary focus was the independent FPY in this study, the Hauser-Feshbach decay calculation also provides more quantities, such as $\bar{\nu}(A)$, $\chi(\nu)$, and $\phi(\gamma)$, whose experimental data should be important constraints on our model. Since the Hauser-Feshbach model will be playing a central role in producing a new FPY data library, extensive discussions on these matters will be made at a forthcoming CRP meeting on Fission Product Yield for the future FPY evaluations organized under IAEA NDS.

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