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ASSESSMENT OF FISSION PRODUCT YIELDS DATA NEEDS IN NUCLEAR REACTOR APPLICATIONS

Kilian Kern, Maarten Becker, Cornelis Broeders*
Institut für Neutronenphysik und Reaktortechnik
KIT Campus Nord
Hermann-von-Helmholtz-Platz 1, 76344 Leopoldshafen, Germany
kilian.kern@kit.edu; maarten.becker@kit.edu; cornelis.broeders@kit.edu

ABSTRACT

Studies on the build-up of fission products in fast reactors have been performed, with particular emphasis on the effects related to the physics of the nuclear fission process. Fission product yields, which are required for burn-up calculations, depend on the proton and neutron number of the target nucleus as well as on the incident neutron energy. Evaluated nuclear data on fission product yields are available for all relevant target nuclides in reactor applications. However, the description of their energy dependence in evaluated data is still rather rudimentary, which is due to the lack of experimental fast fission data and reliable physical models. Additionally, physics studies of evaluated JEFF-3.1.1 fission yields data have shown potential improvements, especially for various fast fission data sets of this evaluation.

In recent years, important progress in the understanding of the fission process has been made, and advanced model codes are currently being developed. This paper deals with the semi-empirical approach to the description of the fission process, which is used in the GEF code being developed by K.-H. Schmidt and B. Jurado on behalf of the OECD Nuclear Energy Agency, and with results from the corresponding author's diploma thesis.

An extended version of the GEF code, supporting the calculation of spectrum weighted fission product yields, has been developed. It has been applied to the calculation of fission product yields in the fission rate spectra of a MOX fuelled sodium-cooled fast reactor. Important results are compared to JEFF-3.1.1 data and discussed in this paper.

Key Words: fission product yields, fission modelling, GEF code, evaluated data, JEFF-3.1.1, fast reactor, sensitivities

1. INTRODUCTION

In the corresponding author's diploma thesis [1] a systematic assessment of fission product analytics is presented. Fission yields depend on the target nuclide, its isomeric state and the kinetic energy of the incoming neutron. State-of-the-art reactor burn-up calculations are performed using fission yields data from evaluated nuclear data libraries, such as JEFF-3.1.1 [2], which is being discussed in this contribution. In these libraries, incident neutron fission yields are provided for the neutron energy range from thermal up to 20 MeV. To account for the neutron energy dependence of fission yields, in JEFF-3.1.1 this energy range is splitted into up to three sub-ranges beginning at thermal energy, 400 keV and 14 MeV, with a fission yields data set ("thermal," "fast" and "high energetic") applying to each of these sub-ranges. Analogously to the provision of multi-group cross-section data, fission yields data are provided in this few-group structure.

*Corresponding author: Kilian Kern

Thermal neutron induced fission has been most extensively studied by experiments. These have been performed in the past e. g. at the Lohengrin and Cosi Fan Tutte spectrometers at ILL Grenoble, where the single nuclide yields and kinetic energies of light fission products have been measured. In the case of fast fission, there are less experiments, different incident neutron energies, mostly incompletely measured mass yield distributions and scarce data on the distribution of isobaric nuclide yields. The latter are also called “fractional independent yields”. This makes the evaluation of fast fission yields rather difficult and motivates the application of a reliable physical fission model. So far, yields measured in experiments with fast reactor spectra have been taken for the evaluation of a single “fast” fission data set, although the neutron energy dependence has been studied in more detail by some experiments. Among fast fission experiments, the incident neutron energy 14 MeV, corresponding to $^2H +^3 H \rightarrow^4 He + n$ fusion neutrons, has been studied more thoroughly [3]. Thus, for some target nuclides a “high energetic” data set is available in JEFF-3.1.1.

With model calculations of fission yields, it is possible to provide finer energy divisions than in existing evaluated data libraries. In this paper the features of GEF (“general fission”) [4], a modern semi-empirical fission model code being developed by K.-H. Schmidt and B. Jurado for the OECD Nuclear Energy Agency, are discussed. The GEFY library [5] contains ENDF-6 formatted fission yields calculated by this code. GEF version 2010/5c has been extended to enable the calculation of spectrum weighted fission yields with an inclusion of multi-chance fission based on existing evaluated cross-section data and also with some changes in the modelling of fragment deexcitation. The extended version is denoted as GEF EXT and has been used to calculate fission yields for fast reactor applications in [1]. Deviations between the calculated yields and the evaluated data have been found which obviously result from an incorrect model description used to complete unknown isobaric nuclide yields in the JEFF-3.1.1 evaluation. Potential applications of the GEF model code in future fission yields evaluations are discussed in section 4.

Deterministic neutronics calculations with 350 energy groups and burn-up calculations have been performed using the modular code system KANEXT [6,7]. The reactor calculations were done on a pin cell scale for a uranium/plutonium MOX fuelled SFR and a uranium/plutonium MOX fuelled PWR for comparison. The characteristics of the obtained fission reaction rate spectra are discussed in subsection 3.2. Furthermore, for the SFR the yields from the GEF EXT calculation have been tested in investigations of the reactivity, the neutron capture characteristics of fission products, the radionuclide inventory of spent fuel and the thermal decay power after reactor shutdown. The results are to be found in [1].

To define two important terms used throughout the paper, it should be mentioned that fission *fragments* are the excited medium-mass nuclei from fission, whereas fission *products* are the final deexcited nuclei after prompt neutron and gamma emission.

2. MODERN SEMI-EMPIRICAL MODELLING OF THE FISSION PROCESS

2.1. Advances in the Modelling of Fission

Since fission fragments can be classified by their masses, N/Z ratios and excitation energies to originate from distinct fission channels, the application of the multichannel theory is a common feature of fission modelling. With this modelling, the fragment mass yields distribution can be well described by a superposition of several Gaussians, which are attributed to the fission channels. According to photofission experiments [8] performed for a wide range of nuclei, the mean charge number of the heavier fragments from the standard 1 and standard 2 channels is relatively constant rather than their mean mass number, as it was assumed in former times [9]. The mean charge numbers are given by (1,2) as a function of the compound nucleus charge and mass numbers Z_{CN} and A_{CN} [4].

$$\overline{Z_{S1,h}} = \frac{70}{3} \cdot \frac{Z_{CN}^{1.3}}{A_{CN}} + 16.5 \tag{1}$$

$$\overline{Z_{S2,h}} = \frac{65}{3} \cdot \frac{Z_{CN}^{1.3}}{A_{CN}} + 21.4 \tag{2}$$

Significant advance in the modelling of the nuclear fission process is made by the explicit application of the so-called "separability principle" [10] in GEF. This principle states that the microscopic potential of a fissioning nucleus is already determined by the shell correction energies of the nascent fragments. There is experimental and theoretical evidence that this principle is applicable not far beyond the outer saddle point of the nuclear potential in deformation space. Calculations based on the Langevin equation of motion show a large inertia for the mass division, but a small inertia for the N/Z ratio of the nascent fission fragments. By assuming the first to be determined at the outer saddle point and the latter at the scission point, one obtains rather good agreements with experimental observations. The application of this principle has the advantage that the knowledge of inertia and friction tensors is not required. Thus, in the modelling of the fission process at first the fission channel and the mass division are chosen. The mean N/Z values of the two fragments may be determined by a scission point model, taking the fragment masses, their deformations and an empirical tip distance between the nuclear surfaces as input. Furthermore, in the GEF code the variances of fragment mass yield distributions and isobaric nuclide yield distributions are also still described on an empirical stage.

It has been found in [1] that the minimization of the liquid-drop potential at the scission point is clearly insufficient to correctly describe the mean N/Z of fission fragments, regardless of the choice of the tip distance. This might be solved by an inclusion of shell effects, whereas the current solution in GEF is to add an empirical shift to the isobaric mean charge numbers, which is $+0.37$ for the lighter and -0.37 for the heavier fragment.

The description of nuclear temperatures and level densities is very important to the prompt neutron emission spectrum, to the division of excitation energy among the two fragments and to even-odd effects in fission fragment yields. Recently, it has been found that for medium-mass nuclei the nuclear temperature stays constant up to an excitation energy of 20 MeV [11], which is explained as the result of a superfluid phase transition in the nucleus. The nuclear temperature in this constant temperature region is well described as a function of mass and shell correction energy.

The GEF code contains a detailed modelling of fission fragment deexcitation, which is based on the Weisskopf-Ewing formalism. In this formalism, the differential decay width of a mother nucleus with excitation energy E and outgoing particle energy E' to a residual nucleus with energy U' is given by (3), with $\omega_{CN}(E)$ and $\omega_n(U')$ the level densities of the mother nucleus and after neutron emission [12]. In (3), $i_n = 1/2$ denotes the neutron spin and μ_n its reduced mass.

$$\widetilde{\Gamma}_n(E, E')\, dE' = \frac{(2i_n + 1)\mu_n}{\pi^2 \hbar^3} \frac{1}{\omega_{CN}(E)} \cdot \sigma_{cn}(E') \cdot \omega_n(U') \cdot E'\, dE' \tag{3}$$

By the application of constant temperature level densities with parameters from von Egidy and Bucurescu [13,14] and the Dostrovsky parameterization (4) for the inverse reaction cross-section (with r_0 the nucleon radius and α, β parameters depending on A), a good agreement of GEF EXT with the evaluated JEFF-3.1.1 prompt neutron emission spectra has been observed in [1]. However, there were still deviations from the experimental prompt neutron numbers, and the general observations point out that a more precise modelling of the competition between neutron and gamma emission needs to be implemented.

$$\sigma_{cn}(E') = \pi r_0^2 \cdot \left(\sqrt[3]{A} + 1\right)^2 \cdot \alpha \cdot \left(1 + \frac{\beta}{E'}\right) \tag{4}$$

In GEF versions 2011/1 or newer, fission fragment spins are also calculated. This is done semi-empirically using an effective moment of inertia being determined by the fragment mass, deformation and excitation energy, the spin of the target nucleus and the excitation energy of the fissioning nucleus as input. The even-odd effect of mean fragment spins depending on the fragment proton number is also included. Using the obtained spin values, the population of isomeric states of fission product nuclides is calculated.

2.2. Fragment Excitation Energies

In order to model prompt neutron emission, even-odd effects in fission fragment yields and the population of isomeric states, a good model description of fragment excitation energies is required. This has only been done by inaccurate approaches up to now. The GEF model code contains a more advanced description in which the nuclear temperatures of fission fragments play an important role. This needs to be explained in some more detail at this point.

The potential energy release E_{sc} up to the scission point is described empirically by (5) with E^*_{CN} the compound nucleus excitation energy, $E_{F,SL}$ the superlong barrier height and Z_{CN}, A_{CN} the proton and mass numbers of the nucleus. The linear dependence of E_{sc} on $\frac{Z^2_{CN}}{\sqrt[3]{A_{CN}}}$ in (5) originates from the work of Asghar and Hasse [15].

$$E_{sc} = 0.08\,\text{MeV} \cdot \frac{Z^2_{CN}}{\sqrt[3]{A_{CN}}} - 93\,\text{MeV} - \begin{cases} E_{F,SL} - E^*_{CN} & E^*_{CN} < E_{F,SL} \\ 0 & E^*_{CN} \geq E_{F,SL} \end{cases} \tag{5}$$

In Schmidt's and Jurado's model [4], the energy brought into the system by the incident neutron is assumed to go into intrinsic excitation, however if it is below the barrier height plus the pairing gap of an even-even fissioning nucleus it is assumed to go into collective excitation. It is further assumed that on the average 40% of E_{sc} ends up in intrinsic and 10% in collective excitation, with the rest going into kinetic energy of the fragments (GEF version 2011-3.7). The collective energy at the scission point is assumed to be equally distributed between both fragments.

For the intrinsic excitation energy, there is a new and original description. With the application of the separability principle, the nascent fragments are assumed to acquire individual nuclear temperatures already on the way between the outer saddle and the scission point. All available intrinsic excitation energy is assumed to flow to the colder (usually the heavier) fragment, with a constant residual energy remaining in the hotter one. With this description, the experimental observation that an increase of the incident neutron energy leads to an increase of prompt neutron emission from the heavier fragment only, can be explained. In older fission models, the intrinsic excitation energy was assumed to be distributed according to the mass ratio of the fragments, which is expected if the nuclear level density is assumed to be a Fermi gas level density. However, this assumption is incorrect for the typical excitation energies of fragments from fission reactions in critical nuclear reactors, which are mostly below 20 MeV. The constant temperatures of the fragments are given by (6) as a function of mass A and shell correction W'. For details, see [1].

$$T = \frac{1}{A^{\frac{2}{3}}} \left(17.45\,\text{MeV} - 0.51 \cdot W'(Z,N) + 0.051 \frac{1}{\text{MeV}} \cdot W'^2(Z,N) \right) \tag{6}$$

After scission, the fragments acquire their ground state deformations, with the deformation energy being released into additional excitation energy. In the GEF code, the initial deformations of fission fragments are taken from a scission point model for the superlong channel, for the standard channels they are either zero at the shell closures or given by empirical linear functions of Z.

It has been observed in experiments at ILL Grenoble that fission fragments with even proton numbers have a higher mean total excitation energy (TXE) than fragments with odd proton numbers. According to Lang et al. [16], the total kinetic energy (TKE) of fission reactions of even-Z nuclei into two even-Z fragments does only follow the enhanced Q value in a superfluid fission process in which the protons stay fully paired. Indeed, in a large fraction of these reactions a proton pair is broken. In this case, the energy for pair breaking is taken from the kinetic energy of the system, resulting in the same TKE as for odd-Z fragments, and a higher TXE. The necessity to include this effect in future GEF versions is discussed in [1].

It is not known from experiments whether there is a similar effect from neutron pair breaking during the fission process. This could have significant impact on the emission of prompt neutrons and should therefore be examined.

2.3. Even-odd Effect of Fragment Yields

The yields of fission fragments before neutron emission, which are generally well described by several Gaussians representing the channel specific fragment mass yields distribution and the isobaric nuclide yields distribution, are modulated by even-odd effects. This effect occurs at compound nucleus excitation energies corresponding to the typical neutron flux spectra of critical nuclear reactors and also in spontaneous fission. The experimental observations are:

- In even-Z fissioning systems, the production of even-Z fragments is generally enhanced regardless of the split asymmetry. However, the enhancement is found to increase with asymmetry.
- In odd-Z fissioning systems, the production of even-Z light fragments and odd-Z heavy fragments is observed to increase with split asymmetry. In rather symmetric splits, no even-odd effect is observed.
- The effect is particularly strong in the fission of e. g. thorium nuclei, and it decreases with increasing proton number of the fissioning nucleus.
- The effect is found to wash out when the excitation energy of the compound nucleus increases.

There have been early attempts to explain this effect via the conservation of proton pairs during the fission process, which however were inconsistent and could e. g. not explain the even-odd effect in odd-Z fissioning systems. Recently, a consistent and physically well-founded description [17], which is connected to the energy sorting mechanism described before, has been found by Schmidt and Jurado.

The global even-odd effect δ is defined by (7) with the total yields of even and odd nuclides Y_{even} and Y_{odd}. In yields as a function of proton or neutron number, locally around a number X_i it is given by (8,9).

$$\delta = \frac{Y_{even} - Y_{odd}}{Y_{even} + Y_{odd}} \tag{7}$$

$$\delta_i = \frac{e^{2\Delta_i} - 1}{e^{2\Delta_i} + 1} \tag{8}$$

$$\Delta_i = \frac{1}{8} \cdot (-1)^{X_i+1} \cdot [\ln Y_{i+3} - \ln Y_i - 3 \cdot (\ln Y_{i+2} - \ln Y_{i+1})] \tag{9}$$

According to Schmidt and Jurado, one needs to distinguish between the even-odd effect originating from pairing correlations and the asymmetry-driven even-odd effect. Both effects depend on the intrinsic excitation energy E^*_{intr} at the scission point. The local proton even-odd effect from pairing correlations is quite well described by the exponential function (10) which takes account of the increase of pair breaking when E^*_{intr} increases.

$$\delta_{pair,p} = e^{-\frac{E^*_{intr}}{4.5\ \mathrm{MeV}}} \tag{10}$$

The asymmetry-driven even-odd effect, on the other hand, is related to the energy sorting process. From the physical point of view, a complete energy sorting between the nascent fragments must include the formation of a fully paired hot fragment (which is usually the light one), since this leads to a higher entropy. This also explains the observed even-odd effect in systems with an odd proton or neutron number. The transfer of a nucleon through the neck of the fissioning nucleus leading to the formation of an even hot fragment is considered as the final step of the energy sorting process. A proton may pass the neck in the time frame before the Coulomb barrier is established, whereas a neutron may pass it until neck rupture. Thus, there will be an asymmetry-driven even-odd effect in the yields if the energy sorting is completed within this time frame. The speed of this energy sorting is assumed to be proportional to the temperature difference $T_{light} - T_{heavy}$ between the nascent fragments.

In the proton number dependent fragment yields of odd-Z fissioning nuclei, there is only the asymmetry-driven even-odd effect, starting at a certain threshold asymmetry of the split. This indicates that the system does not always have enough time to finish the energy sorting before the Coulomb barrier is established. The GEF authors found that the threshold for the occurrence of the asymmetry-driven proton even-odd effect [18] is given by (11).

$$\frac{|T_{light} - T_{heavy}|}{E^*_{intr}} > 0.035 \tag{11}$$

The stochastic nature of the excitation energy and the duration of the energy sorting leads to a gradual increase of the even-odd effect with asymmetry. The interference of pairing correlations δ_{pair} with the asymmetry-driven even-odd effect δ_{asym} can be described by the empirical relation (12), with $|\delta_{asym}| \leq 1$ [4]. As shown in [17], with this model description the coarse characteristics of proton even-odd effects in fission product yields are well reproduced for a number of nuclides.

$$\delta = \delta_{pair} + (0.5 - \delta_{pair}) \cdot \delta_{asym} \tag{12}$$

The even-odd effect in neutron number dependent fragment yields is described analogously. Unfortunately, the neutron number dependent yield distribution before evaporation is experimentally unknown. Assumptions with respect to the characteristics of the neutron even-odd effect have to be made, which influence post-neutron fission product yields and prompt neutron multiplicities. This is still a source of uncertainty in the modelling.

3. REACTOR PHYSICS APPLICATIONS

3.1. Reactor Calculations

The calculations of reactor neutronics and burn-up have been performed with the modular code system KANEXT [6,7], developed in the past four decades at today KIT Campus Nord. It is capable of performing deterministic neutronics calculations with up to 350 energy groups. Good descriptions of the available options and of input specifications may be found in references [19,20]. The calculation of burn-up is based on the principles of the original ORIGEN code [21], which has been extended for application in the BURNUP module and in the external KORIGEN code [22]. The reactor calculations were carried out on a representative homogenized pin cell basis for a SFR design with uranium/plutonium MOX fuel and a fissile content of 11.7%. This design originates from a recent proposal in an international project [23]. For comparison to the SFR, fission reaction rates for a uranium/plutonium MOX fuelled PWR with a fissile content of 6.0% are presented in section 3.2. With this PWR MOX fissile content, the pin cell reaches a final burn-up of about $40\frac{\text{GWd}}{\text{t}_{\text{hm}}}$. The pin cell specifications of the PWR design have been adopted from [24], and the plutonium vector was taken from the calculation of a 4.65% enriched uranium cycle in the same cell, with a burn-up of $40\ \frac{\text{GWd}}{\text{t}_{\text{hm}}}$, assuming six years of cooling time before and one year of storage after the refabrication. The plutonium vectors are given in Table I, and the bulk of the fuel is depleted uranium. Each calculation was performed in 350 energy groups.

Table I. BOC Fuel Compositions of the SFR and the PWR Cell [at%]

	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am
SFR	1.96	52.94	25.49	9.80	7.84	1.96
PWR	1.90	60.16	22.58	10.09	4.78	0.49

3.2. Fission Reaction Rates

Neutron flux spectra and energy-dependent fission rates have been investigated with KANEXT. In this context, one finds that also in a SFR, fission reaction rates of thermally fissile nuclides are concentrated at incident neutron energies below about 100 keV, whereas thermally non-fissile nuclides like ^{238}U show a threshold behaviour. Table II lists the fraction of fission reactions above a neutron energy of 400 keV for the fuel nuclides for which a “thermal” fission yields data set is provided in the JEFF-3.1.1 library. It shows that, in comparison to a PWR, in a SFR the “fast” fission yields data set applies to a larger fraction of the fission rates of thermally fissile nuclides. In relation to this, it should be noted that the total fission rate fraction to which the high-quality JEFF-3.1.1 “thermal” data sets apply is only 58.5% in the SFR, but 89.3% in the PWR.

Table II. Weight of Fast Fission ($>$ 400 keV) for Specific Nuclides

Target	Fission reaction rate fraction above 400 keV $[\%]$	
	SFR	PWR
^{235}U	17.6	3.8
^{238}Pu	42.6	42.1
^{239}Pu	27.7	3.3
^{241}Pu	18.0	2.3
^{241}Am	94.0	65.4

In this work, the obtained fission rate spectra have been condensed into equidistant 10 keV bins and plotted in a double linear scale, which is more relevant for the physical effects of the fission process. The integral fission rates within the range where the “fast” fission data sets apply have been normalized to one, and the plots are shown in Figs. 1 - 2.

To provide calculated fission yields data for a specific energy range from E_a to E_b, a spectral weighting needs to be performed. This energy weighting of fission yields $Y(Z, N, I, E)$ with the proton, neutron and isomeric state numbers Z, N, I of the fission product and the incident neutron energy E for a specific neutron flux spectrum $\varphi(E)$ is done by (13).

$$\overline{Y}(Z, N, I) = \frac{\int_{E_a}^{E_b} dE\, Y(Z, N, I, E) \cdot \sigma_f(E) \cdot \varphi(E)}{\int_{E_a}^{E_b} dE\, \sigma_f(E) \cdot \varphi(E)} \tag{13}$$

Within the relatively narrow energy range to which the "thermal" data set applies, i. e. up to 400 keV, the sensitivities of the weighted fission yields $\overline{Y}(Z, N, I)$ to the different fission rate spectra are expected to be very small. However, within the energy range where the "fast" fission yields data sets of JEFF-3.1.1 apply, one also finds significant deviations between the fission rate spectra of the two reactor types. Surprisingly, the different scattering characteristics of the coolant lead to a harder flux spectrum for the PWR within this energy range, resulting in the fission rates shown in Figs. 1 - 2. Nevertheless, compared to the PWR, the SFR flux spectrum is considerably enhanced in the range from 5 keV to 700 keV, which enables more fission of nuclides like ^{238}Pu whose fission barrier is only slightly higher than its neutron binding energy. The deviating fission rate spectra of the two reactors, as shown in the diagrams, can be expected to significantly affect the yields $\overline{Y}(Z, N, I)$ of sensitive nuclides, weighted over the "fast" energy range.

With the current data structure of JEFF-3.1.1, the deviations between the weighted yields for the "fast" energy range will not be reproduced in reactor calculations, and a more detailed description of the energy dependence of fission yields in nuclear databases is desirable.

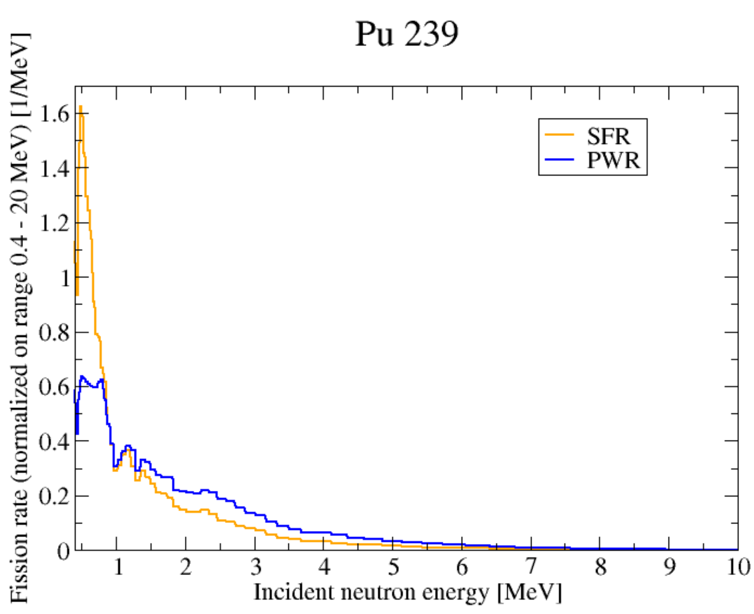

Figure 1. Fission Reaction Rate of $^{239}\mathrm{Pu}$ per Unit Energy, Condensed on 10 keV Bins

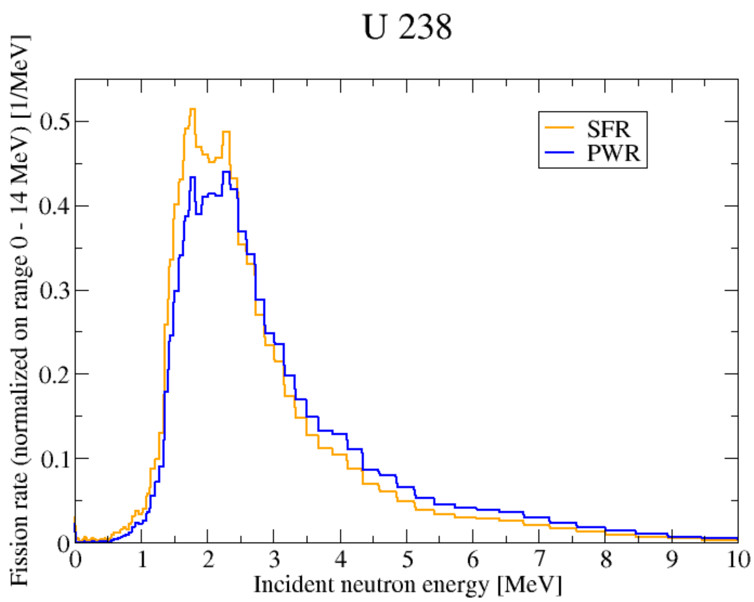

Figure 2. Fission Reaction Rate of ^{238}U per Unit Energy, Condensed on 10 keV Bins

3.3. Fission Yields Calculations

With the extended code version GEF EXT, spectrum weighted fission yields have been calculated for the SFR fission reaction rates obtained from the neutronics calculation, according to (13). When comparing the fission yields predicted by the code to the “fast” fission data sets of JEFF-3.1.1, one notices a discrepancy regarding the even-odd effect of fission product proton numbers. The yields in Figs. 3 - 4 have been calculated for the fission reaction rates to which these data sets apply. In the JEFF-3.1.1 data, there is always only a small even-odd effect originating from the application of Wahl’s empirical “Z_p” model in the evaluation [25], which is in conflict with the prediction of GEF EXT. Regarding this effect, there is a definite potential to improve future evaluated nuclear data libraries by the application of the more advanced and physically well-founded model from Schmidt and Jurado. The discrepancy between Wahl’s Z_p model and their description of the even-odd effect is rather large in the case of nuclides with lower Z, such as thorium and uranium isotopes, whereas for higher Z nuclides like plutonium isotopes the discrepancy decreases. The predictions from the GEF EXT code are also confirmed by a $^{238}U(\gamma, f)$ photofission experiment [26], in which a global even-odd effect of $\delta_p = 0.200$ in the proton number dependent yields was observed at a mean compound nucleus excitation energy of 8.3 MeV, corresponding to an incident neutron energy of 3.5 MeV in this case. According to subsection 2.2, the additional neutron of the $^{238}U(n, f)$ fissioning nucleus lowers the intrinsic excitation energy gain up to the scission point by only 61 keV. In the JEFF-3.1.1 data, the global proton even-odd effect of $^{238}U(n, f)$ fast fission yields is only $\delta_p = 0.055 \pm 0.018$. Above all, these deviations could have an impact on the characteristics of beta decay power and delayed neutron emission, but this has not yet been investigated.

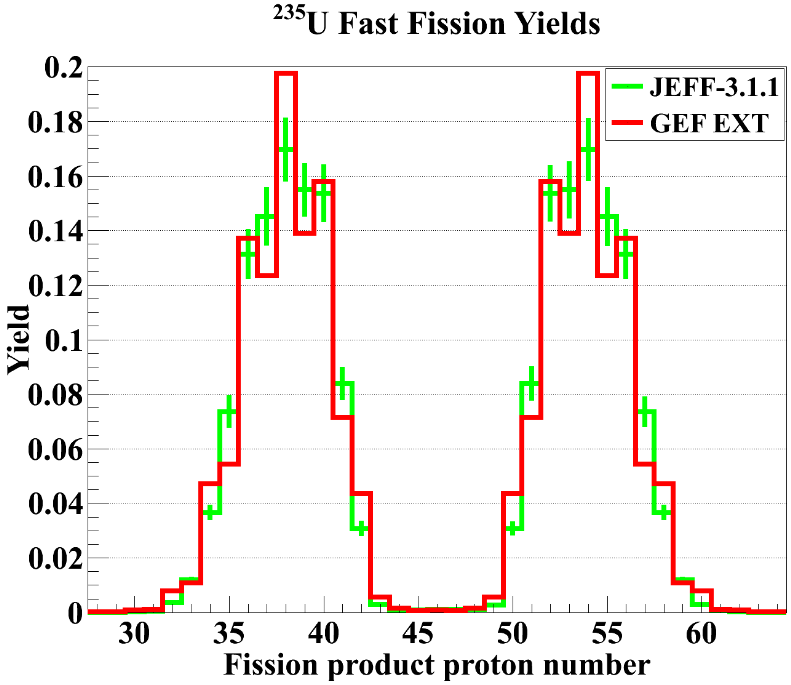

Figure 3. Calculated Fast Fission Yields of ^{235}U vs. JEFF-3.1.1 Data

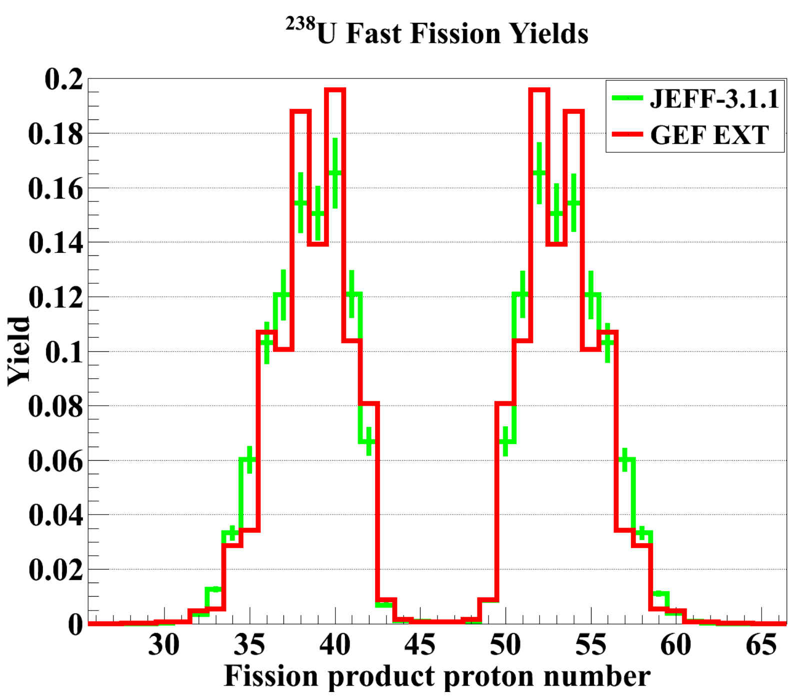

Figure 4. Calculated Fast Fission Yields of ^{238}U vs. JEFF-3.1.1 Data

4. POTENTIAL MODEL APPLICATIONS IN FUTURE FISSION YIELDS EVALUATIONS

As discussed before, the GEF code can be useful for creating a new, improved evaluation of fission yields data. Nevertheless, in the evaluation of nuclear data it will have to be carefully applied, since the precise modelling of the fission process still faces several challenges. The most important ones are the correct modelling of the single fission channel fractions, the fission fragment excitation energies and the deexcitation of fission fragments by neutron and gamma emission.

The modelling of even-odd effects in fission product nuclide yields is the most likely application of the GEF code in a nuclear data evaluation. For a given fission product mass with an unknown isobaric nuclide yield distribution, one may want to take this entire distribution from the model code. The important neutron energy sensitivities of fission product yields discussed in the last section are expected to be mainly related to their mass distribution. However, for a correct completion of unknown yields of isobaric nuclides, the entire nuclide yields distribution has to be modelled correctly.

One should ensure that the measured mass yields distribution and prompt neutron emission are well reproduced, and that the modelled fission yields are consistent with the observed radioactive decay and delayed neutron emission characteristics. A model with sufficient predictive power for the mean proton numbers and variances of the isobaric yield distributions will be needed.

With a good modelling of mass yields and prompt neutron emission, unknown mass yields could also be estimated in an advanced way. In the GEF code, the standard 3 fission channel which shows up in the fission of plutonium or higher element isotopes, is also included. Its characteristics are, however, not yet well understood.

The GEF model code could also enable a better estimate of unknown isomeric ratios of fission products. In the JEFF-3.1.1 evaluation, a model from Madland and England was applied [25], which only takes the spins of ground and isomeric states as input. In the GEF model, on the other hand, fragment spins are calculated including newest physical insight, whereas a full Hauser-Feshbach deexcitation model still needs to be established (as of October 2011). The quality of the calculated isomeric ratios has not been investigated in this work.

5. CONCLUSION

The development of the GEF code shows that with new physical insight and original approaches, a relatively good and simple modelling of the fission process can be achieved. These approaches especially involve the separability principle, the “energy sorting” process and the even-odd effect of fragment yields related to it. It has been shown that there is a potential to better include the neutron energy dependence of fission product yields in reactor burn-up calculations. In the case of a fast reactor, JEFF-3.1.1 data sets, whose evaluation was less based on experimental data and had to rely more on model descriptions, become important. The application of Wahl’s Z_p model in the evaluation is questionable at least with respect to the even-odd effect of fission product nuclide yields. This problem could rather easily be solved by an application of the GEF code. It should be investigated how the yield distributions among isobaric fission product nuclides affect the various reactor physics observables.

Concerning the JEFF-3.1.1 evaluation and the GEF code, it can be summarized that an application of GEF in fission yields evaluations is motivated by several interesting features of the code. These are the original description of even-odd effects in fission fragment yields, the modern calculation of fragment excitation energies and spins and the detailed assessment of fragment deexcitation. The model could be applied to improve even-odd effects, isobaric yield distributions or even the mass yield distributions in evaluated fission yields data. The GEF code could also be used for the calculation of unknown isomeric ratios of fission product nuclides. However, some work on fission modelling remains to be done. Several physical effects are not yet well understood, empirical descriptions are necessary, and assumptions on effects with little experimental insight have to be made. The purpose of the GEF code is to provide a high predictive power for a wide range of fissioning nuclei, and for a single nucleus current versions still require several adjustments.

The aim of the corresponding author is to develop a new version of GEF EXT with applicability to a wider range of nuclides, based on a newer GEF version. An ENDF-formatted library of calculated fission yields in the KANEXT energy group structure is going to be created, which will enable precise studies of the sensitivities of the weighted yields $\overline{Y}(Z, N, I)$ to the reactor specific neutron flux spectrum.

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