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Preliminary Results of a Full Hauser-Feshbach Simulation of the Prompt Neutron and Gamma Emission from Fission Fragments

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Abstract

The prompt neutron and gamma emission from fission fragments are investigated through the Monte Carlo code FIFRELIN which is developed at the CEA Cadarache research center. In a previous release of the code, the de-excitation of the fragments was treated in a two steps process. First the emission of all the prompt neutrons was simulated using a Weisskopf spectrum for the distribution of their kinetic energy. In a second step, the excitation energy still available was dissipated by the fragments as an electromagnetic decay cascade. This paper presents a new procedure for fragment de-excitation using an Hauser-Feshbach treatment of prompt particles emission. The neutron/gamma competition is then accounted for during the whole cascade. Moreover, the neutron emission is now ruled by the transmission coefficients directly coming from an optical model calculation performed with TALYS-1.4. The implementation of these models in the code FIFRELIN is quickly highlighted. The results in terms of neutrons and gamma multiplicities and spectra for one simulation of a ^{252}Cf spontaneous fission are emphasized. The neutron multiplicity experimental data are used to constraint the parameters of our simulation. The prompt gamma spectrum calculated is then consistent with experimental data and the structures observed experimentally in the low energy range are well reproduced. However, the same simulation performed with several different nuclear models and parameters reveals high variation of these fission observables. For example, the average total gamma energy $\langle E_{\gamma, \text{tot}} \rangle$ is shown to vary up to 20% with changes in the level density or radiative strength function model.

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1. Introduction

The conception of new designed PWR with massive steel reflector made the gamma heating problematic a burning issue. The high accuracy requests, in terms of evaluated nuclear data, for coupled neutron-gamma transport calculation motivate us to study more deeply the fission fragments de-excitation process. In this work, the Monte Carlo code FIFRELIN (Litaize and Serot, 2010) which is developed at the CEA Cadarache research center is used to perform simulations of fission fragments de-excitation cascades. In the previous releases of the code, the emission of prompt particles from one fragment was treated in a two steps calculation (Regnier et al., 2013). All the prompt neutrons were

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emitted first and their kinetic energy in the center of mass frame were sampled in a Weisskopf spectrum. Then excitation energy still available was dissipated as an electromagnetic decay cascade. This paper presents a new procedure for fragment de-excitation using an Hauser-Feshbach treatment of prompt particles emission. The neutron/gamma competition is accounted for during the whole cascade. Moreover, the neutron emission is now ruled by the transmission coefficients directly coming from an optical model calculation performed with TALYS-1.4 (Koning et al., 2011). This paper presents the main ideas of the Hauser-Feshbach cascades implementation in the code FIFRELIN. The preliminary results in terms of neutrons and gamma multiplicities and spectra from the simulation of a ^{252}Cf spontaneous fission are highlighted. At last, the sensitivity of these main observables to several nuclear models and parameters is investigated.

2. The Hauser-Feshbach treatment of the fragments de-excitation in FIFRELIN

The FIFRELIN device aims to simulate the fission fragments evaporation process using Monte Carlo methods and statistical models of the nucleus. The simulation consists in the realization of a great number of fission events (typically 10^5 events). Estimators for fission observables are incremented during each event.

The first step in the simulation of one fission event consists in the generation of the two fully accelerated primary fragments. In this phase, their nuclear mass number and kinetic energy are sampled using experimental yields. Their charge and total angular momentum are sampled from empirical laws. Typically, the probability distribution of the primary fragments spin is given by:

$$P_{L,H}(J) \propto \frac{(2J+1)}{2\sigma_{L,H}^2} e^{-\frac{(J+1/2)^2}{2\sigma_{L,H}^2}} \quad (1)$$

where $\sigma_{L,H}^2$ is the spin cutoff of the distribution for the light (L) or heavy (H) fragment. The total excitation energy available at this stage of the fission (TXE) is divided between the two fragments following:

$$TXE = a_L T_L^2 + E_{rot,L} + a_H T_H^2 + E_{rot,H} \quad (2)$$

where $a_{L,H}$, $T_{L,H}$, $E_{rot,L,H}$ stands for the level density parameter, the nuclear temperature and the rotational energy of the fragments respectively. In this preliminary work, we assumed a null rotational energy for both fragments. An empirical mass dependant law is used for the temperature ratio $R_T = \frac{T_L}{T_H} = f(A)$. In this work, this law is composed of two linear functions and is driven by two parameters $R_{T,min}$ and $R_{T,max}$ (see Ref. (Litaize and Serot, 2010) for details).

Knowing the properties of the fully accelerated fragments (A , Z , E^* , J , π), the de-excitation process is then simulated in the framework of the Hauser-Feshbach statistical model (Hauser and Feshbach, 1952). Its implementation in FIFRELIN is based on the knowledge of a complete level scheme of the fragment up to an energy limit. This energy is chosen so that the level density is equal to 10^5 levels per MeV. Below this energy limit, a complete discrete level scheme is determined using a process already described in Ref. (Regnier et al., 2012). Experimental levels coming from the RIPL-3 (Capote et al., 2009) database are taken into account. Above the energy limit, the detail of discrete levels is no more computed and the decay algorithm relies on average nuclear properties over 10 keV energy bins. Knowing the level scheme and the initial excited level i of a primary fragment, the code is able to calculate the decay probability to every reachable level or bin f . These probabilities are either given by experimental data from RIPL-3 or in most cases calculated. Both neutron and gamma emissions are considered possible from the beginning of the de-excitation and the probability to decay from the discrete level i to a reachable discrete level f can be expressed via the partial widths of the transition ($\Gamma(i \rightarrow f, \dots)$):

$$P_p(i \rightarrow f, \dots) = \frac{\Gamma_p(i \rightarrow f, \dots)}{\Gamma_\gamma^{tot} + \Gamma_n^{tot}}, \quad p = n, \gamma \quad (3)$$

The gamma partial width are calculated using the radiative strength function $f_{XL}(\epsilon_\gamma)$:

$$\Gamma_\gamma(i \rightarrow f, XL) = \frac{f_{XL}(\epsilon_\gamma) \epsilon_\gamma^{2L+1} y_{fluctuation}}{\rho(E_i, J_i, \pi_i)}, \quad (4)$$

where $y_{fluctuation}$ accounts for the Porter-Thomas fluctuation and is sampled in a χ^2 distribution with one degree of freedom.

If the neutron emission channel is open, its partial width is not null and can be calculated by the formula:

$$\Gamma_n(i \rightarrow f, l, j) = \frac{T_{l,j}(\epsilon_n) y_{fluctuation}}{2\pi\rho(E_i, J_i, \pi_i)} \quad (5)$$

where $T_{l,j}(\epsilon_n)$ are the neutron transmission coefficients provided by a TALYS-1.4 optical model calculation.

The probability to reach a final bin (above the energy limit) is obtained by summing Eq. 3 over the final levels contained in the bin. Based on this probability distribution, a transition is sampled and the excited nucleus gets to a new level or bin. The same algorithm is repeated until a stable or metastable level of the fragment is reached.

3. Calculation example for a ^{252}Cf spontaneous fission

Using the algorithm described previously, a calculation of 2.10^5 events of ^{252}Cf spontaneous fission has been lead. A Koning-Delaroche spherical potential was used to calculate the neutron transmission coefficients with TALYS-1.4. This calculation example relies on the composite Gilbert-Cameron level density model. The enhanced generalized Lorentzian model as described in RIPL-3 was chosen for the E1 gamma strength function. The numerical main parameters of the calculation are the spin cutoff of the total angular momentum distribution of both fragments and the extremum values of the temperature ratio $R_T(A)$. They were arbitrary set in order to obtain a fair agreement between the calculated and experimental neutron multiplicity $\bar{\nu}$ and its distribution $\bar{\nu}(A)$. The numerical values of these parameters are the following ones:

$$\sigma_H = 10.3\hbar, \quad \sigma_L = 8.6\hbar, \quad R_{T,max} = 1.4, \quad R_{T,min} = 0.6$$

3.1. Prompt neutron observables

The average values obtained for the prompt neutron multiplicity are reported in Table 1. The statistical error (1σ) is less than 0.2% for these estimators. The choice of our parameters implies a global agreement between the calculated neutron multiplicity quantities and the experimental data. However, one can notice on Fig. 1, a trend to overestimate the heavy fragment neutron multiplicity in the very asymmetric fragmentations range.

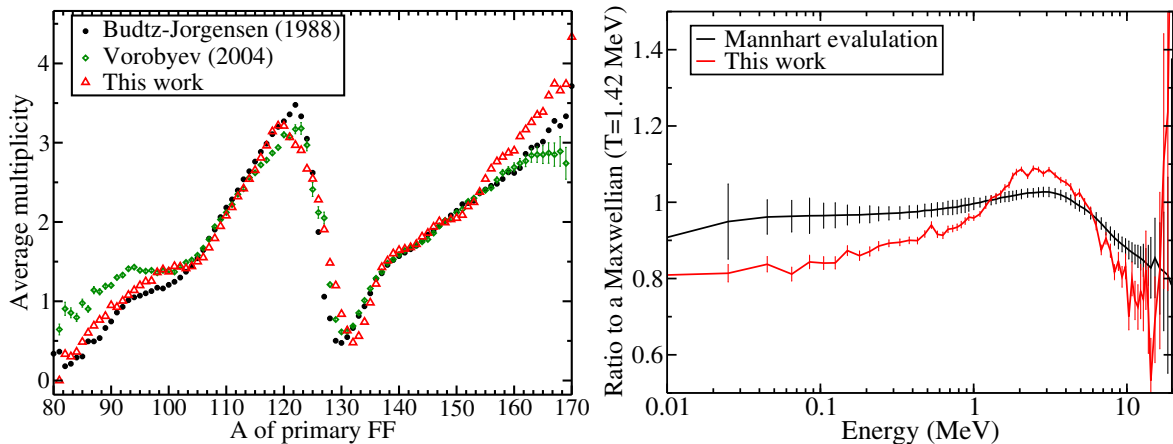


Fig. 1. (left hand side) Average neutron multiplicity versus primary fragment mass; (right hand side) Ratio of the normalized neutron spectrum to a Maxwellian with $T=1.42$ MeV

Concerning the prompt neutron spectrum in the laboratory frame, Fig. 1 shows that our calculation reproduces the evaluation of Mannhart (Mannhart, 1987) up to 10 MeV within roughly 15% of relative deviation.

Table 1. Neutron observables from spontaneous fission of ^{252}Cf

Reference	$\bar{\nu}_{tot}$ (n/f)	$\bar{\nu}_H$ (n/f)	$\bar{\nu}_L$ (n/f)
Vorobyev et al. (Vorobyev et al., 2004)	3.76 ± 0.03	1.70	2.05
This work	3.75	1.73	2.02

3.2. Prompt gamma observables

The average total energy dissipated as prompt gamma rays $\langle E_{\gamma,tot} \rangle$ as well as the average prompt gamma multiplicity \bar{M}_γ are given in Table 2. In order to compare these results with experimental data, the energy threshold in gamma detection must be taken into account. Several experimental data obtained with a detection energy threshold between 60 and 150 keV have been reported in Table 2. The corrected values of multiplicities and total gamma energy coming from FIFRELIN have been calculated without taking into account gamma-rays under 150 keV. This calculation reproduces the order of magnitude of the gamma observables. The total energy available for prompt gamma emission seems to be overestimated by several 100 keV compared to most of the experimental data. This might be caused by an underestimation of the neutron total width or by an overestimation of the gamma total width during the cascade simulation.

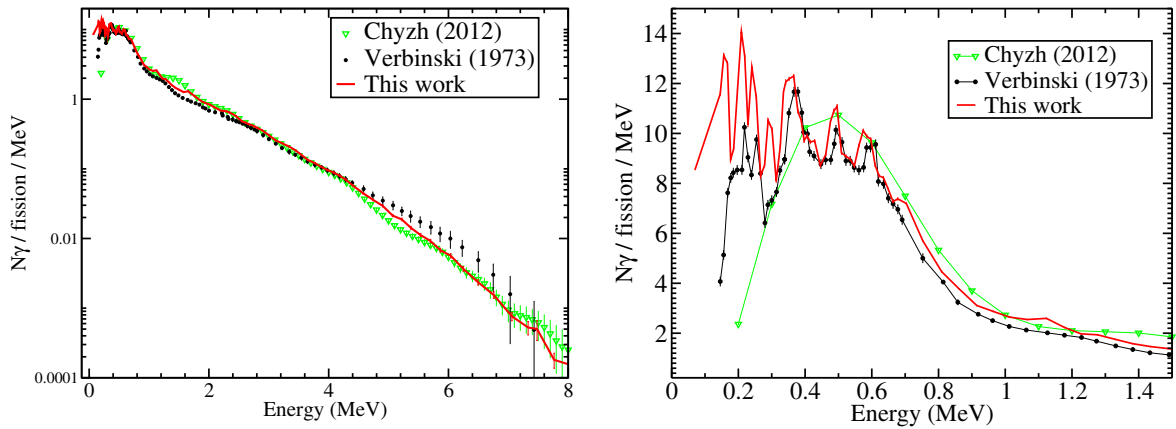


Fig. 2. Prompt gamma spectrum in the laboratory frame (same resolution as Verbinski measurements)

Table 2. Survey of the prompt gamma from spontaneous fission of ^{252}Cf

Reference	Detection threshold (keV)	\bar{M}_γ (γ/f)	$\langle E_{\gamma,tot} \rangle$ (MeV/f)
Smith et al. (Smith et al., 1956) (1956)	60	10.3	8.2
Verbinski et al. (Verbinski et al., 1973) (1973)	140	7.80	6.84 ± 0.3
Nardi et al. (Nardi et al., 1973) (1973)			6.7 ± 0.4
Skarsvag (Skarsvag, 1980) (1980)	114	9.76 ± 0.4	6.99 ± 0.3
Chyzh et al. (Chyzh et al., 2012) (2012)	150	8.16 ± 0.4	7.8^a
Billnert et al. (Billnert et al., 2013) (2012)	100	8.30 ± 0.08	6.64 ± 0.08
This work	0	10.4	7.8
This work	150	9.1	7.7

^a derived from $\langle E_{\gamma,tot} \rangle = \langle \epsilon_\gamma \rangle \bar{M}_\gamma$

The prompt gamma spectrum in the laboratory framework is shown in Fig. 2 and is consistent with the experimental data up to 8 MeV. A fine comparison of the structures of the spectrum at low energies has been realized using the Verbinski (Verbinski et al., 1973) experimental energy grid. As the fragments are not stopped in the sample in the Verbinski experimental setup, the Doppler effect must be taken into account when calculating the spectrum in the

laboratory frame. We assumed in this work that the fragments did not lose energy in the sample and that the gamma emission was isotropic in the fragment frame. Then a Lorentzian transformation enables us to determine the spectrum in the laboratory framework. As can be seen in Fig. 2, the three main structures observed by Verbinski are reproduced by our calculation.

4. The nuclear models and parameters influence

In the RIPL-3 database, several empirical formula as well as microscopic calculation results are described for the level densities, the radiative strength functions, and the optical model potentials. In order to emphasize the impact of the choice of these models in our simulation, several calculations with various combination of models have been performed. The level density models managed by our code are the constant temperature model (CTM), the composite Gilbert-Cameron model (CGCM), and RIPL-3 tabulated values provided by Hartree-Fock-Bogoliubov calculation (HFB). The strength function models used were the standard Lorentzian (SLO), the enhanced generalized Lorentzian (EGLO) and also tabulated values coming from microscopic calculation (HFB). At least, two different optical models potential have been tested for the calculation of the neutron transmission coefficients: the Koning-Delaroche (KD) potential and the Jeukenn-Lejeune-Mahaux (JLM) one.

The variations of the main fission observables induced by a change in the nuclear model used are reported in Table 3. The reference calculation is the one presented in section 3. These results show the high sensitivity of both neutron and gamma observables to the level density. It seems also that the reference calculation overestimates the total gamma energy compared to the other set of nuclear models. The slope of the high energy part of the prompt gamma spectrum is also impacted by the choice of the level density and the E1 strength function.

A preliminary sensitivity study of fission observables to the four main parameters of the simulation (σ_H , σ_L , $R_{T,max}$, $R_{T,min}$) have been lead. It seems that the level of the prompt gamma spectrum below 0.8 MeV is essentially ruled by the two spin cutoff of the fragments spin distribution. A work is in process to improve the methodology used to set the values for these parameters.

Table 3. Variation of fission observables due to different modelisations of one physical quantity. The reference calculation uses the CGCM, KD, EGLO set of nuclear models.

Nuclear models used			Relative variation from reference (%)				
Level density	Optical model	E1 Strength function	$\bar{\nu}$	$\langle\epsilon_{n,Lab}\rangle$	\bar{M}_γ	$\langle E_{\gamma,tot}\rangle$	$\langle\epsilon_\gamma\rangle$
CTM	KD	EGLO	-3.0	-20.8	+18.9	+5.5	+8.0
HFB	KD	EGLO	-2.4	+6.0	+8.0	-15.7	-4.4
CGCM	JLM	EGLO	-2.8	+9.3	-0.2	-18.4	+0.1
CGCM	KD	SLO	-0.3	+0.2	-3.0	-18.2	+3.4
CGCM	KD	HFB	+0.8	+0.1	-7.7	-20.6	+5.4

5. Conclusion

In that work, the implementation of a full Hauser-Feshbach treatment of the fission fragments de-excitation in the code FIFRELIN is highlighted. This modelisation takes into account the neutron/gamma competition. An example of calculation performed for the ^{252}Cf spontaneous fission gives us a set of fission observables that are compared to experimental data. Neutron multiplicity experimental data have been used to constraint the model parameters. The calculation produces gamma observables comparable with recent experiments even if the average total energy seems to overestimate most of the available experimental data by several 100 keV. Concerning the prompt gamma spectrum, the global shape obtained is consistent with experimental data. Moreover, the structures in the low energy range that were observed by Verbinski and confirmed by the work of A. Oberstedt et al. (Billnert et al., 2013) are reproduced by our calculation. A first sensitivity study of this calculation to the nuclear models choice for level density, strength function and optical model potential emphasizes variations of the main fission observables up to 10-20%. Among the numerous perspectives to this work, a methodology to determine the best values for the four main parameters of our calculation is in process.

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