New results in the modeling of fission and radiative neutron capture with FIFRELIN

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Abstract. The FIFRELIN Monte Carlo code has been upgraded recently by adding new capabilities, additional models and updated databases. Several examples are presented in this work as well as three different applications related to the prompt component in fission, gamma cascades from thermal neutron capture and the delayed component in fission associated to the time evolution of decay heat.

1 Introduction

This work aims at showing improvements performed in the FIFRELIN Monte Carlo de-excitation code. New results related to fission observables as well as single gamma cascades after thermal neutron capture will be discussed. General upgrades are described in section 2 and three different applications will be presented such as the prompt fission gamma-ray multiplicity as a function of mass in the case of ^{252}Cf spontaneous fission (section 3), gamma cascades from thermal neutron capture in ^{155,157}Gd isotopes (section 4) and the delayed fission component through the time evolution of the decay heat after a ^{235}U(n$_{th}$,f) reaction burst (section 5).

2 Brief overview of code upgrade

Since the last general publication regarding the FIFRELIN code [1] several modifications, improvements, new data handling as well as new capabilities are now available in the code. Most of them will be briefly summarized below:

- Basic input data, as described for instance in [2], are the pre-neutron mass yields as well as the first and second moments of the gaussian disctribution of the Fission Fragment (FF) kinetic energy as a function of mass. It is now possible to handle a 2D matrix Y(A,TKE) directly from experiments or to use the primary mass, charge and kinetic energy results obtained from the GEF code [3].

- Nuclear charge can be sampled from two different parametrizations of Wahl's model [4, 5].

- Internal conversion coefficients for electron emission are used from the RIPL-3 database at low energy (as usual) but to fill the gap they are now also tabulated from the BrIcc code [6] up to 6 MeV as a function of nuclear charge, electron shell and sub-shells as well as multipolarity. Mixing ratios are also taken into account.

- Tabulated nuclear level densities $\rho(E, J, \pi)$ from microscopic + combinatorial calculations (Hartree-Fock-Bogoliubov HFB formalism) are now available in the code. FIFRELIN can use level densities based on a Skyrme effective interaction (BSk14) [7] taken from RIPL-3, as well as level densities based on a Gogny effective interaction (D1M) [8].

- Microscopic photon strength functions for electric and magnetic dipole transitions (D1M+QRPA) [9] are now available, directly taken from the TALYS code [10].

- A complete refactoring of the ROOT [11] package used to analyze FIFRELIN events has been undertaken, increasing its capabilities.

- Gamma angular correlations can be accounted for using statistical tensor theory [12] in gamma cascades after thermal neutron capture and are in progress for fission calculation considering different alignment hypothesis of the primary fragment spins.

- The EGAF database [13] for thermal neutron capture cascades (handling ENSDF database is in progress) can be used for specific applications as described in section

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4. If the primary transitions are not fully known from EGAF, a 'mixed calculation route' can be performed with a 'theoretical' FIFRELIN calculation and an 'experimental' EGAF cascade with the appropriate weighting.

- A coupling has been done between FIFRELIN and the PHITS+DCHAIN (JAEA) system code [14, 15] allowing to deal with delayed components in fission and especially time evolution of decay heat as discussed in section 5.

3 Prompt fission observables: focus on multiplicities

It has been shown recently that the average prompt gamma multiplicity as a function of mass $\bar{M}_\gamma(A)$ has a saw-tooth shape (as for neutrons) [16]. This was measured for the spontaneous fission of ^{252}Cf with the VESPA spectrometer from EC-JRC (Geel, Belgium) involving a double Frisch-grid ionisation chamber and an array of LaBr$_3$(Ce) detectors. FIFRELIN calculations were able to reproduce this trend using a composite Gilbert Cameron level density model (CGCM) as described in [17] and an energy dependent spin cutoff parameter (EDS), entering the primary FF total angular momentum distribution (this EDS parametrization was successfuly initiated in [18]). In our previous work [16] the shape of $\bar{M}_\gamma(A)$ was reasonable, the magnitude (i.e. the total average multiplicity $\bar{M}_\gamma$) was not and required a renormalization to the experimental γ-ray multiplicity. The use of a HFB+BSk14 microscopic nuclear level density model [7] allows us to reproduce the saw-tooth shape and magnitude of both neutron and gamma-ray multiplicities as a function of pre-neutron mass [19], as illustrated in Fig. 1.

Table 1. Calculated average multiplicities (neutron values are target ones) for the ^{252}Cf(sf) reaction. Statistical uncertainties in FIFRELIN calculations are lower than 0.01.

Neutron multiplicities	$\bar{\nu}_L$	$\bar{\nu}_H$	$\bar{\nu}$
Vorobyev et al. [20]	2.05	1.70	3.76(3)
FIFRELIN	2.07	1.70	3.76
Gamma multiplicities	$\bar{M}_\gamma^L$	$\bar{M}_\gamma^H$	$\bar{M}_\gamma$
Travar et al. [16]	4.53(3)	3.83(3)	8.36(2)
FIFRELIN	4.66	3.70	8.36

This was done in a single consistent calculation with one set of free parameters: $R_T^{78} = 0.5$, $R_T^{132} = 1.45$, $f_\sigma^L = 1.4$ and $f_\sigma^H = 1.3$, where the R_T parameters drive the initial excitation energy of primary fragments and f_σ are scaling factors that drive their initial total angular momentum. These four free parameters were selected for reproducing a set of chosen target observables, which are the measured neutron multiplicities from Ref. [20]. A higher spin for light fragments is considered compared to heavy ones in order to reproduce the average gamma multiplicity as a function of mass. This is consistent with recent theoretical studies [21]. Average neutron and gamma multiplicities are presented in Table 1. The reader will find additional details in [19].
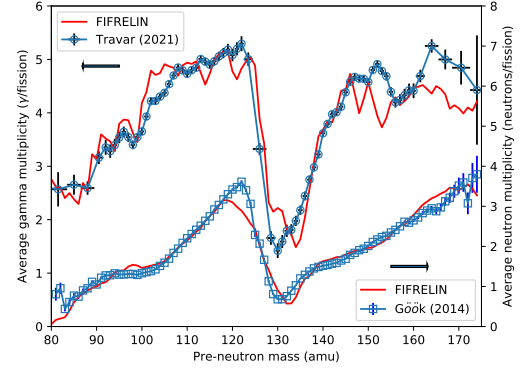

Figure 1. Average neutron and gamma multiplicities as a function of pre-neutron mass for the spontaneous fission of ^{252}Cf.

4 Thermal neutron capture cascades

The FIFRELIN code can be used to simulate the de-excitation of any nucleus by neutron, gamma and conversion electron emission. Cascades after thermal neutron capture, have been recently calculated for several nuclei in the field of neutrino research through the STEREO [22] and CRAB [23] projects. Regarding the STEREO reactor anti-neutrino experiment, cascades from ^{155}Gd(n$_{th}$, γ) and ^{157}Gd(n$_{th}$, γ) reactions are used to improve the calculation of the efficiency through the energy deposited in a cell containing a gadolinium loaded liquid scintillator. The aim of STEREO is to test the sterile neutrino hypothesis. The Inverse Beta Decay process (IBD) is considered: $\bar{\nu}_{e-} + p \rightarrow n + e^+$. An anti-neutrino hits a proton to generate a positron and a neutron that will suffer collisions in the scintillator down to thermal energy and then will be captured by gadolinium isotopes. The resulting gamma cascade in coincidence with the positron signal is the signature of an anti-neutrino. The calibration is performed with AmBe sources where (α, n) reaction is used to generate neutrons and a precise cascade is mandatory for deducing systematic uncertainties. Generation of Gd-cascades in GEANT-4 for STEREO simulations was initially performed with a model called GLG4sim, inherited from past neutrino experiments. However this model did not allow for an accurate reproduction of the calibration spectra.

A first and major improvement has been obtained by replacing Gd-cascades calculated with GL4sim with the ones calculated with FIFRELIN [22]. A second improvement has been made possible by considering a mixing of EGAF database for primary transitions from the entry state (S_n, J, π) and theoretical FIFRELIN calculations. A final improvement comes from the $\gamma - \gamma$ angular correlations implemented in FIFRELIN events root tree using statistical tensor theory [12].

Figure 2 shows an example of such a correlation for ^{156}Gd. The reconstructed energy spectrum is shown in Fig. 3. The flat shape of the ratio Data/MC (where 'MC' stands for the GLG4Sim Monte Carlo simulation using FIFRELIN cascades and 'Data' stands for the measurement) allows a good control of the detection efficiency [22]. The reader will find more details in [24].
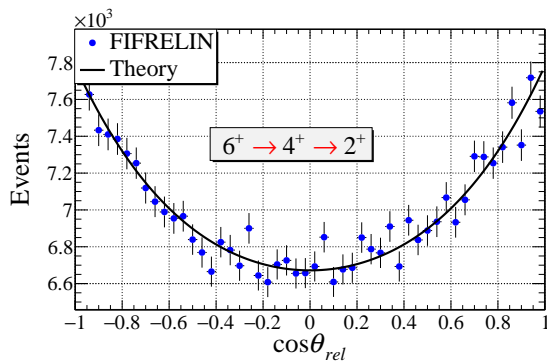
Figure 2. $\gamma - \gamma$ angular correlation for the $6_1^+ \rightarrow 4_1^+ \rightarrow 2_1^+$ cascade in ^{156}Gd used for the validation of the statistical tensor theory implemented in FIFRELIN [12].
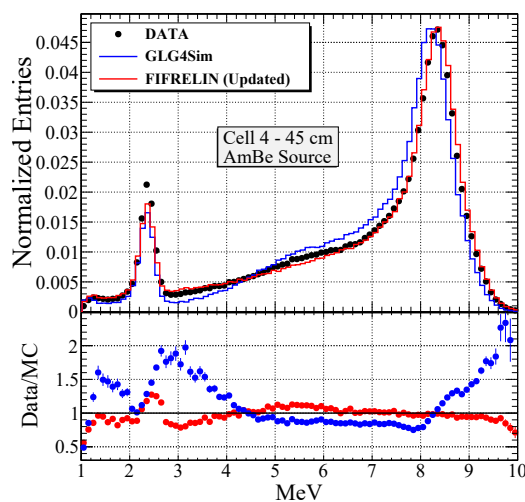

Figure 3. Reconstructed energy spectrum of the STEREO detector in coincidence with 4.4 MeV prompt γ-ray from an AmBe source placed at the calibration position of cell 4 (at about the half the height of the cell). The comparison is performed between GLG4Sim and FIFRELIN involving EGAF primary cascades and γ-γ correlations.

5 Delayed fission observables: focus on decay heat

By default, FIFRELIN calculates the whole set of prompt fission observables and a rough estimation of the average delayed neutron multiplicity by simply accounting for the number of neutrons emited when a $\beta^- n$ level is reached after a prompt cascade. Here, the code has been interfaced with the DCHAIN-PHITS [14] general purpose radiation transport code [25]. Indeed, isotopic fission yields can be provided by FIFRELIN to DCHAIN-PHITS. The DCHAIN burn-up functionality of the PHITS transport code calculates the nuclide inventory and decay heat, among other, based on the activation and decay data libraries through the Bateman equation. In this work, total and gamma decay heat from 0.2 to 10^5 s after a ^{235}U(n$_{th}$,f) burst are shown in Fig. 4 and compared with data compilations from Dickens [26] and Tobias [27]. Before the code upgrade (from FIFRELIN-2018 to FIFRELIN-2021),

neutron rich Rb, Sr, Cs and Ba isotopes were systematically overproduced (see Fig. 6 of ref [25]). In this work, the nuclear charge distribution from the Wahl's Z_p model are modified to account for the revision in Ref. [5], pre-neutron mass yields come from [28] and finally the RIPL3-2020 release of the nuclear structure database is accounted for, improving the calculated decay heat over the whole time range for the thermal fission of ^{235}U (FIFRELIN-2021 in Fig. 4). All these modifications allow to reduce the overestimation observed with the previous FIFRELIN-2018 calculation, up to roughly 100 s. Fission fragments having longer half-lives are no longer overestimated. For more details, the reader can refer to Ref. [25].
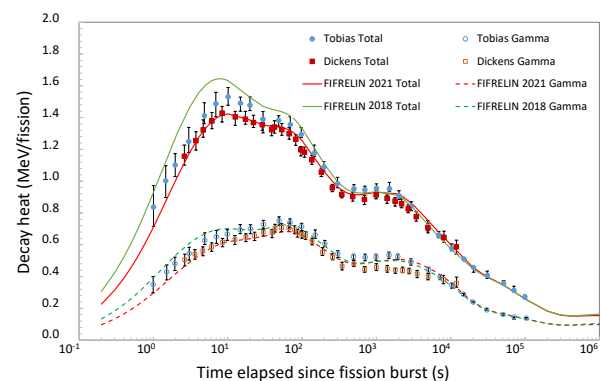

Figure 4. Decay heat after neutron burst (^{235}U(n$_{th}$,f)) calculated with FIFRELIN and DCHAIN-PHITS system code and compared with Tobias [27] and Dickens [26] for gamma and total (gamma + electron) components.

6 Conclusion

Some recent improvements performed in the FIFRELIN code have been briefly presented, such as new pre-neutron data format for FF mass and kinetic energy or nuclear charge models, a new release of the nuclear structure database, interfacing with GEF or PHITS-DCHAIN codes, use of microscopic level densities and photon strength functions as well as $\gamma - \gamma$ angular correlations.

Calculations obtained with this new release are in good agreement with experimental data such as VESPA for prompt fission gamma-ray observables, STEREO for gamma cascades after thermal neutron capture and time evolution of the decay heat after ^{235}U burst. Additional improvements and studies are in progress such as particle correlations in fission or the interfacing with ENSDF database.

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