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Modeling Pu-239 Fission Fragment De-Excitation applying the Total Monte Carlo method in TALYS

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Abstract. In this study, we applied the Total Monte Carlo (TMC) methodology in de-excitation simulations of primary fission fragments (FF) using the TALYS code. The goal was to develop and optimise a methodology to benchmark initial fission model assumptions on fission mass yield distributions, excitation energy sharing and angular momentum population. The study was performed on the thermal neutron induced fission of ^{239}Pu(n$_{th}$,f). The work aimed at evaluating fission model deficiencies and parameter sensitivities. We systematically varied TALYS input data by generating 5000 random files through the GEF code, randomizing 94 model parameters that affect fission yields and energy distributions within 3% of their default values. This variation revealed significant changes in the fission observables, such as prompt neutron and γ-ray multiplicities and energy spectra. The results indicate some systematic defects in the assumed excitation-energies and angular momenta. Another outcome from the study is the identification of a need for new correlation measurements on prompt neutrons and γ-rays from the ^{239}Pu(n$_{th}$,f) reaction, as well as an updated evaluation.

1 Introduction

In nuclear fission, excited fission fragments emit prompt neutrons and γ rays during de-excitation. Data from these emission processes are vital for nuclear technology and for modeling of the fission process. Key parameters include fission product yields, neutron and γ-ray multiplicities, and the energy spectra of prompt neutrons and γ rays. Modelling these observables is complex, especially when varying fission systems and energies. Current research focuses on predicting correlations in fission data, especially where empirical data is lacking. To address challenges in modeling nuclear fission data a new feature was added to the well-known TALYS [1] reaction code, allowing it to simulate the full nuclear de-excitation of a predefined list of nuclides and calculate relevant evaporation data. This customization enables users to create tailored databases for direct comparison between simulated and experimental data, essential for validating mass yields, energy sharing, and angular momentum. A proof-of-principle study [**?**] used the GEF [3] code to generate 737 databases for various nuclei and excitation energies, benchmarking them against experimental data. While the results were generally satisfactory, discrepancies were noted in the prompt fission neutron spectrum and even more profoundly in the γ-ray emission characteristics. A sensitivity study [4, 5] explored the impact of TALYS parameter adjustments on evaporation data, but it did not change initial conditions like fission yields or excitation energies. To investigate the influence of systematics uncertainties in these input parameters, the current work introduces random perturbations to the fission-model parameters within the GEF code and generates varied databases as input to the TALYS code [6]. This methodology is a step towards a Total Monte Carlo (TMC) [7] approach to quantify sensitivities of de-excitation results to such perturbations.

2 Method

The GEF model includes 94 adjustable fission parameters, making uncertainty analysis quite complex. The TMC method simplifies this by implicitly accounting for correlations between parameters, facilitating the uncertainty analysis [7]. We implemented the TMC method in the current study by extending the built-in GEF function 'MyParameters' to allow for perturbation of all 94 GEF parameters, and used it to create varied databases for TALYS [6]. 5000 randomly perturbed data sets for fission fragment yields ($Y_{\mathrm{ff}}(Z, A)$), the average excitation energies ($\overline{E^*}$) and their standard deviations (σ_{E^*}), along with the average total excitation energies ($\overline{TXE}$) and average total kinetic energies ($\overline{TKE}$), were created by drawing parameter values from a normal distribution centered on the GEF parameter default values, with σ = 3%. For parameters with a default value of 0, σ was set to 0.03. TALYS determines the evaporation process of the perturbed files using a Hauser-Feshbach model [1, 9]. To integrate these perturbed files with TALYS, a new keyword was introduced into the TALYS source code to manage the file names and input data [6].

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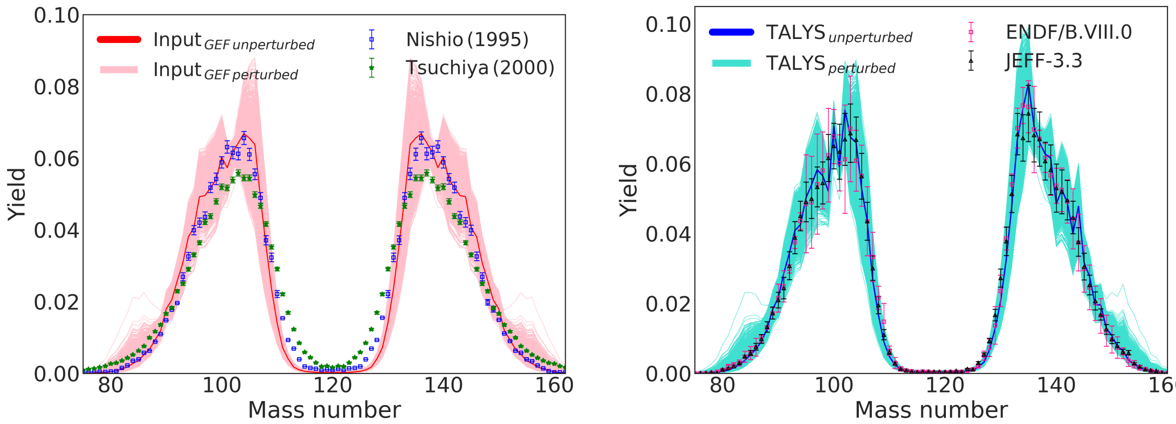

Figure 1. Left: The pre-neutron emission mass yields for ^{239}Pu(n_{th},f), from GEF used as input to TALYS, in comparison with experimental data from [11, 14]. Right: The post-neutron mass yields calculated by TALYS in comparison to evaluated data from [13, 15].

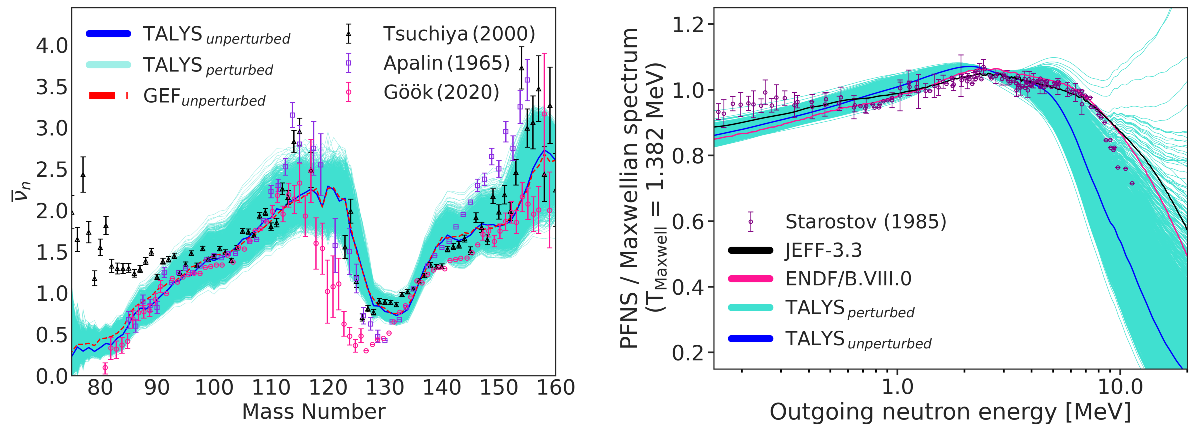

Figure 2. Left: The average prompt fission neutron multiplicity ($\bar{\nu}_n(A)$) for ^{239}Pu(n_{th},f), from TALYS for the default GEF input files and the 5000 random files [3, 10? , 11]. Right: The prompt fission neutron spectrum (PFNS) is calculated as a ratio to a Maxwell distribution in the form $f_M = (2\sqrt{E}/(\sqrt{\pi}T^{3/2}))\exp(-E/T)$, at a temperature $T = 1.382$ MeV, together with data from Refs. [13, 15, 16].

3 Results

The developed methodology involves generating random files with GEF and subsequently de-exciting the fission fragments using TALYS [6]. This approach has recently been applied on ^{235}U(n_{th},f) [8]. In this work we employed the methodology on the ^{239}Pu(n_{th},f) reaction. Figure 1 shows the fission product yields determined by TALYS (right), derived from 5000 random GEF input files (left). The results reveal notable fluctuations in yields, particularly around the peak regions of the standard-1, standard-2, and super-asymmetric fission modes.

The average number of prompt fission neutrons, $\bar{\nu}_n(A)$, exhibits a saw-tooth trend due to fragment shell effects, as shown in Fig. 2 (left). Comparison of the default and perturbed TALYS results with experimental data shows that, in the light mass region, the TALYS calculations are closer to the data from Refs. [10] and [?], while for heavier masses, the results align more with the data from Tsuchiya et al. [11]. It is clear that the experimental data are in disagreement, partly owing to poorer energy resolution and lacking corrections for neutron recoils, as pointed out by Göök et al. [?]. Note especially the strong shift around double-magicity ($A = 132$). Therefore there is an eminent need for further experimental investigation.

The prompt fission neutron spectrum (PFNS) is shown in Fig. 2 (right), as a ratio to a Maxwell distribution with a temperature of $T = 1.382$ MeV, as adopted from Ref. [16]. The TALYS PFNS is generally softer compared to the other spectra. A few random files appear to enhance the spectrum, but not at both low and high energies simultaneously.

Figure 3 displays the distributions of the average total neutron and γ-ray multiplicities, as well as the average neutron and γ-ray energies from both GEF and TALYS. Table 1 provides a summary of the averages of the distributions in comparison with the GEF and TALYS default values, which are indicated by the dashed lines in Fig. 3.

The average neutron multiplicity values from the perturbed files show a slightly better agreement with the evaluated data files from ENDF and JEFF. The standard deviation (spread) in the neutron values from the random files is $\sigma(\bar{\nu}) \approx 0.15$, which is a large effect. The average en-

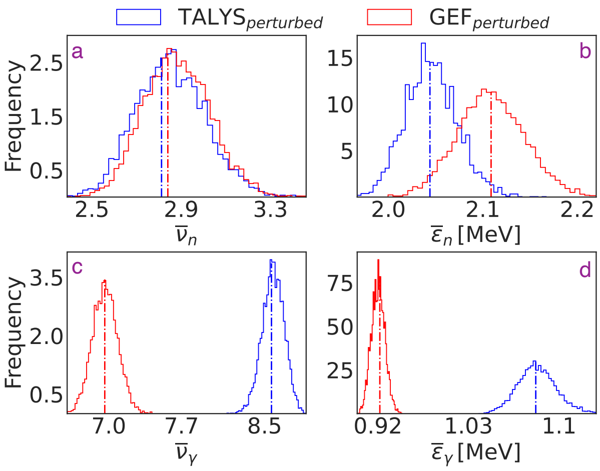

Figure 3. The evaporation results following the 5000 random files. a) The average number of emitted prompt fission neutrons b) the average energy per prompt neutron c) the average number of prompt fission γ-rays and d) the average energies per γ ray. The dashed lines denotes the default values.

Table 1. Summary of evaporation data from ^{239}Pu(n_{th}, f)

Prompt fission-neutron multiplicities and energies				
Code	$\bar{\nu}_n$	σ_{ν_n}	$\bar{\epsilon}_n$ [MeV]	σ_{ϵ_n} [MeV]
GEF$_{unperturbed}$	2.84		2.11	
GEF$_{perturbed}$	2.88	0.15	2.11	0.04
TALYS$_{unperturbed}$	2.81		2.04	
TALYS$_{perturbed}$	2.85	0.16	2.05	0.03
ENDF/B.VIII.0	2.87		2.12	
JEFF-3.3	2.86		2.12	
Prompt fission γ-ray multiplicities and energies				
Code	$\bar{\nu}_\gamma$	σ_{ν_γ}	$\bar{\epsilon}_\gamma$ [MeV]	σ_{ϵ_γ} [MeV]
GEF$_{unperturbed}$	6.96		0.96	
GEF$_{perturbed}$	6.97	0.12	0.96	0.01
TALYS$_{unperturbed}$	8.57		1.08	
TALYS$_{perturbed}$	8.58	0.11	1.08	0.01
ENDF/B.VIII.0	7.56		0.84	
JEFF-3.3	7.90		0.80	

ergy per neutron is rather underestimated in TALYS and the spread in the energy is quite small.

The average total γ-ray multiplicities differ significantly. GEF underestimates the average number of γ-rays, whereas TALYS shows a higher multiplicity, compared to the evaluated data. The standard deviation following the random files is around $\sigma(\bar{\nu}_\gamma) \approx 0.12$. Both codes predict a higher average γ-ray energy compared to JEFF and ENDF.

4 Conclusions and outlook

We applied the TMC methodology in de-excitation calculations of primary fission fragments using GEF as input generator to TALYS. The study was performed on the ^{239}Pu(n_{th},f) reaction. All 94 model parameters in the GEF code were randomly varied (σ=3%) to produce random input files for TALYS. In summary, TALYS and GEF exhibit a closer agreement on prompt fission neutron data compared to prompt γ-rays. The level of TMC randomization applied proved to be quite significant, causing substantial fluctuations in the average evaporation data.

This study indicates that the ^{239}Pu(n_{th},f) reaction requires renewed focus and additional experimental campaigns. The observed neutron multiplicity and energy spectrum exhibit considerable discrepancies compared to theoretical predictions and existing evaluations.

Moving forward, we intend to concentrate on the specific parameters that influence how excitation energy is shared between the two nascent fragments.

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