FIFRELIN – TRIPOLI-4® coupling for Monte Carlo simulations with a fission model. Application to shielding calculations

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Abstract. TRIPOLI-4® Monte Carlo transport code and FIFRELIN fission model have been coupled by means of external files so that neutron transport can take into account fission distributions (multiplicities and spectra) that are not averaged, as is the case when using evaluated nuclear data libraries. Spectral effects on responses in shielding configurations with fission sampling are then expected. In the present paper, the principle of this coupling is detailed and a comparison between TRIPOLI-4® fission distributions at the emission of fission neutrons is presented when using JEFF-3.1.1 evaluated data or FIFRELIN data generated either through a n/γ-uncoupled mode or through a n/γ-coupled mode. Finally, an application to a modified version of the ASPIS benchmark is performed and the impact of using FIFRELIN data on neutron transport is analyzed. Differences noticed on average reaction rates on the surfaces closest to the fission source are mainly due to the average prompt fission spectrum. Moreover, when working with the same average spectrum, a complementary analysis based on non-average reaction rates still shows significant differences that point out the real impact of using a fission model in neutron transport simulations.

1 Introduction

Monte Carlo transport calculations including fission sampling usually use nuclear data from international evaluation libraries such as JEFF-3.1.1 or ENDF/B-VII.1. Among those data, fission multiplicities for neutrons and gamma are provided only as mean values instead of a probability distribution function depending on the incident neutron energy, as observed physically. Moreover, the neutron emission spectrum may be restrictive since it is provided as a function of the incident neutron energy only and is thus the same for all fission neutrons produced by a given fission event. Consequently, when using these data in a Monte Carlo transport code, the energy conservation is preserved in mean value only, but not for each individual fission event.

On the contrary, fission models such as FIFRELIN [1] or FREYA [2] give access to a detailed simulation of the fission, including particle correlations and energy conservation. In the past, several works aimed at coupling various fission models with Monte Carlo transport codes or at integrating them, for example MCNP-DSP [3], MCNPX-PoliMi [4] or FREYA-TRIPOLI-4® [5]. Related calculations were mainly dealing with nuclear instrumentation applications for which individual events are collected and post-processed. However, in the context of shielding calculations in fission facilities, spectral effects of the use of a fission model for specific isotopes could be first analyzed in terms of average values provided by the Monte Carlo transport code. Secondly, an analysis based on non-average distributions could be performed in order to observe correlation effects between fission neutrons for example. These issues are addressed in the present paper by means of the TRIPOLI-4® [6] Monte Carlo transport code and the FIFRELIN fission model.

TRIPOLI-4® is a continuous-energy Monte Carlo transport code dedicated to shielding, reactor physics with or without depletion, criticality safety and nuclear instrumentation. A first coupling between TRIPOLI-4® and FREYA fission model has already been implemented [5] and consists in calling FREYA code by TRIPOLI-4® at each sampling of a fission event. In order to test another fission model, a new coupling with FIFRELIN code has recently been implemented starting from version 10 of TRIPOLI-4® code and works through external files between both codes.

FIFRELIN is a Monte Carlo code that simulates the de-excitation process of primary fission fragments leading to an estimation of prompt fission observables such as neutron/gamma/electron multiplicities and spectra in correlation with fission fragments. Primary fission fragments (after full acceleration and before prompt neutron emission) are completely determined by the knowledge of their mass A, charge Z, kinetic energy KE, excitation energy E* and spin/parity J^{π}. The three first characteristics (A, Z, KE) are sampled from experimental data or can be provided by external codes. The description of the initial (E*, J) entry zone is

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performed through a mass dependent temperature ratio law $R_T(A)$ and a spin/parity distribution ruled by a spin cut-off parameter that can be modeled in different ways. Positive and negative parities are supposed to be equally likely. More details can be found in [7].

De-excitation cascades are simulated following the Becvar's notion of nuclear realization [8]. A nuclear realization is a random set of nuclear levels (energy, spin, parity) in association with partial widths for neutron, gamma or electron emission. Experimental data related to electromagnetic transitions in the discrete level region are taken from RIPL-3 database [9]. When nuclear level structure is completely unknown (in the continuum region), level density and strength function models are used. In between these regions, our partial knowledge of nuclear structure is completed by models up to a fixed maximum level density. In this way the whole available experimental information is accounted for.

FIFRELIN is ruled by five free input parameters driving the primary fission fragment excitation energy and spin-parity distributions (the (E*, J) entry zone discussed above). These five free parameters are determined to match a target observable such as the total average prompt neutron multiplicity (nu-bar). Once this procedure is completed, the whole set of fission observables can be compared with experimental results. The cascade can be modeled in two different modes, either *n/γ-uncoupled* or *n/γ-coupled*. In the first mode, neutron emission is modeled from Weisskopf statistical theory down to a spin dependent energy limit and gamma emission uses nuclear realization concept down to the ground state. The second mode is based on a Hauser-Feshbach formalism accounting for the competition between neutron and gamma emission at the very beginning of the cascade [10]. In this case the neutron emission is ruled from transmission coefficients tabulated on a specific energy-angular momentum grid. The nuclear realization concept is then extended for neutron emission up to the initial fragment excited state.

The purpose of this paper is to present the coupling details and give a preliminary application analyzing the impact of the use of FIFRELIN model on a TRIPOLI-4® shielding calculation including fission sampling. To meet this need, the ASPIS benchmark [11] was selected with several simple modifications for the purpose of this work. Section 2 of this paper is dedicated to the principle of the present coupling and Section 3 to its application to the modified ASPIS benchmark and to further investigations.

2 Coupling method

2.1 General principle

As already mentioned, the FIFRELIN-TRIPOLI-4® coupling was carried out through external files per fissile isotope of interest and therefore works in two consecutive steps: first, FIFRELIN code is run to produce a large amount of fission events for a given fissile isotope. For each fission event, specific data are stored in an output file that can be read by TRIPOLI-4® afterwards. This step can be repeated independently for several fissile isotopes of interest. Then, during the Monte Carlo neutron transport simulation, whenever a fission event needs to be sampled, TRIPOLI-4® reads the data stored in the appropriate FIFRELIN file, if it exists, at the current reading position for a new fission event (otherwise the evaluation files are used). Fission neutrons are directly produced accordingly in TRIPOLI-4® instead of sampling the number of fission neutrons and their energy and angle according to the evaluation distributions. The FIFRELIN files are read sequentially and need therefore to be as big as possible for each fissile isotope of interest, in order to provide as many statistically independent fission events as possible. Then, the fission neutrons carry on with their history through the usual neutron transport simulation of TRIPOLI-4®.

2.2 Validity and contents of a FIFRELIN file

The actual FIFRELIN list-mode (event-by-event) data file is simplified to contain an even number of lines (two lines for a fragment pair). Each line contains the nuclear charge, the mass number, the initial fragment kinetic energy, the characteristics of the cascade and the final (post-neutron) fragment kinetic energy. The characteristics of a cascade depend on the calculation scheme. In the n/γ-uncoupled mode it contains the neutron kinetic energy for every emitted neutron, while in the n/γ-coupled mode it contains the energy, spin and parity of every nuclear level and the kinetic energy in the laboratory frame of every neutron, gamma and conversion electron. In a very first step the emission is supposed to be isotropic in the laboratory frame. These events can be used to estimate a distribution like the prompt fission neutron spectrum allowing a comparison with estimators available in the code.

The nuclear realization concept is very time consuming. Because we were only interested in neutron emission, we started this work by using the n/γ-uncoupled mode and cut out gamma emission. Multi-threading was used to generate 2.10^8 fission fragment cascades on 100 threads for ^{235}U in the thermal incident neutron energy range. This prevented the use of a same history in the subsequent TRIPOLI-4® run.

Then, in a similar way, we used the n/γ-coupled mode to simulate around 4.10^7 fission fragment cascades. Even if gammas are not useful here, partial neutron and gamma widths have to be estimated to account for n/γ competition during the cascade. The major models used in this calculation scheme are:

- Koning-Delaroche optical model potential parametrization for neutron transmission coefficients
- Composite Gilbert-Cameron model for the level density taking into account an energy dependent Ignatyuk level density parameter
- Enhanced Generalized Lorentzian for E1 photon strength functions and Single Lorentzian for other multipolarities.

All these models and model parameters are described in RIPL-3 documentation [9].

2.3 Related distributions as retrieved by TRIPOLI-4®

As expected, using FIFRELIN instead of evaluated data induces modifications to the fission neutron multiplicity distribution and to the fission neutron spectrum. To make this clear, for both modes of FIFRELIN we compared several distributions related to fission neutron emission, obtained with two TRIPOLI-4® simulations (using either FIFRELIN data or JEFF-3.1.1 library) and involving thermal neutron induced fission on ^{235}U. Three quantities of interest were collected by specific TRIPOLI-4® tallies which do not take into account neutron transport simulation. Figure 1 compares prompt fission neutron multiplicities, Figures 2 and 3 present prompt fission neutron spectra and Figure 4 shows the distributions of the energies summed up for all neutrons emitted at a same fission event. Error bars are not presented since they are not visible in terms of orders of magnitude, compared to the displayed values. In the captions, "Fifrelin n" stands for the n/γ-uncoupled mode and "Fifrelin n/γ" for the n/γ-coupled mode of FIFRELIN.

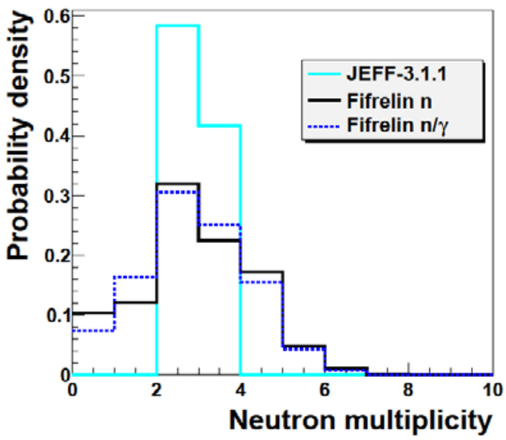

Fig. 1. Prompt fission neutron multiplicity distribution.

In Figure 1, the fission neutron multiplicity distribution obtained with FIFRELIN data spreads from 0 up to 9 neutrons emitted per fission event (with an average value of 2.431 for the n/γ-uncoupled mode and 2.413 for the n/γ-coupled mode) whereas only 2 or 3 fission neutrons can be emitted simultaneously when using the evaluated data (which corresponds to both integer numbers surrounding $\overline{\nu_p} = 2.417$ for ^{235}U at thermal incident neutron energies).

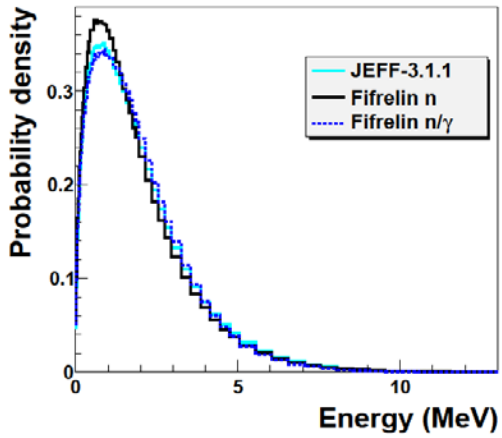

Fig. 2. Prompt fission neutron spectrum.

In Figure 2, the emission spectrum for fission neutrons is slightly shifted to lower energies when using FIFRELIN data based on the Weisskopf statistical theory, i.e. n/γ-uncoupled mode. A prompt spectrum with similar features would be obtained when using FREYA code [5], which also uses Weisskopf statistical theory for neutron emission. Moreover, the emission spectrum looks closer to the evaluated data in case of the Hauser-Feshbach formalism of FIFRELIN, i.e. n/γ-coupled mode. However, the lin-log representation of these spectra shows a slight discrepancy noticeable in Figure 3 at energies higher than approximately 2 MeV.

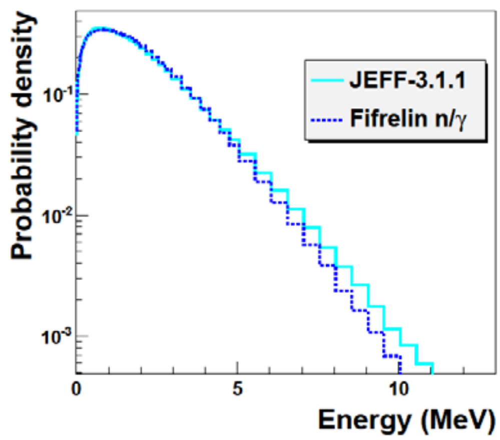

Fig. 3. Prompt fission neutron spectrum, lin-log representation.

Average values of these spectra are 2.035 MeV with JEFF-3.1.1 data and 1.943 MeV with the n/γ-uncoupled mode or 1.984 MeV with the n/γ-coupled mode of FIFRELIN.

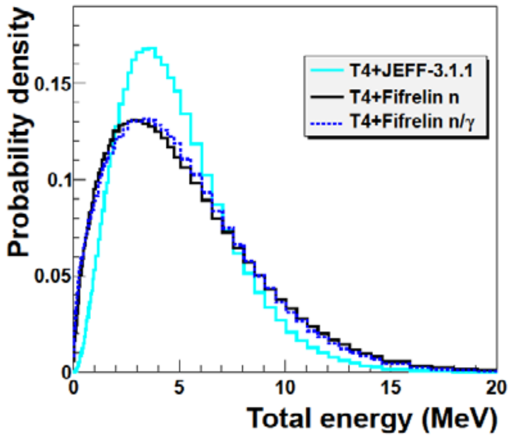

Fig. 4. Sum of neutron energies per fission.

The distributions plotted in Figure 4 are clearly not centered on the same energy: the distribution obtained with the evaluated data turns out to be more peaked and centered on a higher energy. Average values of these distributions are 4.907 MeV with JEFF-3.1.1 data and 4.720 MeV with the n/γ-uncoupled mode or 4.781 MeV with the n/γ-coupled mode of FIFRELIN. The impact of this difference after transport of the fission neutrons is investigated in the next Section.

3 Application to thermal ^{235}U in a fixed-source ASPIS calculation using FIFRELIN data

3.1 Description

We have selected the ASPIS benchmark from the SINBAD Database [11]. This configuration allows us to study the propagation of neutrons with energies higher than 40 keV from a fission plate into an iron bulk. Three different dosimeters are installed at various depths of penetration (from 5 cm to 1.2 m):

- ^{103}Rh(n,n'), threshold = 40 keV
- ^{115}In(n,n'), threshold = 339 keV
- ^{32}S(n,p), threshold ≈ 1.6 MeV.

Reaction rates are calculated for all these dosimeters.

Several modifications were made on this benchmark for the purpose of this study. With the aim of simulating fission events, a 10 eV-source was placed in the fission plate (instead of the usual Watt-spectrum together with fission sampling turned off).

When running TRIPOLI-4® with FIFRELIN data or with the evaluated data, the same following options were activated. Fission sampling was turned on, as well as the analog transport mode of the code [12]. No variance reduction was requested, in order to avoid an underestimation of the fission sampling. Finally, only prompt fission neutrons were sampled.

3.2 Results

No significant increase of the calculation time was noticed (less than 1%) when running TRIPOLI-4® with FIFRELIN data instead of the evaluated data for the fission sampling on ^{235}U, provided that the ahead calculation time of FIFRELIN is not taken into account. Tables 1 to 6 compare average surface neutron reaction rates in arbitrary units (a.u.) calculated by three simulations of the modified ASPIS benchmark, either using JEFF-3.1.1 library or n/γ-uncoupled mode of FIFRELIN (Tables 1, 3 and 5), or n/γ-coupled mode of FIFRELIN (Tables 2, 4 and 6), respectively on ^{103}Rh (Tables 1 and 2), ^{115}In (Tables 3 and 4) and ^{32}S (Tables 5 and 6) IRDF85 nuclei. Only results on the surfaces closest to the fission plate are shown. Relative standard deviations are given in percentages and relative errors of FIFRELIN results are presented in numbers of sigma, with reference to the JEFF-3.1.1 results. It should be noted that the convergence was better for the n/γ-uncoupled mode, due to a higher total number of fission events present in the related FIFRELIN files.

Table 1. Comparison of TRIPOLI-4® reaction rates on ^{103}Rh when using JEFF-3.1.1 or FIFRELIN n/γ-uncoupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-uncoupled	Rel. err. (nb. σ)
5.72	51.786 ± 0.101	50.525 ± 0.081	19.1
11.43	30.347 ± 0.095	29.731 ± 0.099	14.9
17.15	18.798 ± 0.128	18.395 ± 0.115	12.5
22.86	12.023 ± 0.133	11.807 ± 0.136	9.6
28.58	7.879 ± 0.156	7.756 ± 0.152	7.3
34.29	5.300 ± 0.180	5.217 ± 0.165	6.5

Table 2. Comparison of TRIPOLI-4® reaction rates on ^{103}Rh when using JEFF-3.1.1 or FIFRELIN n/γ-coupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-coupled	Rel. err. (nb. σ)
5.72	51.786 ± 0.101	51.743 ± 0.126	0.5
11.43	30.347 ± 0.095	30.335 ± 0.155	0.2
17.15	18.798 ± 0.128	18.722 ± 0.184	1.8
22.86	12.023 ± 0.133	12.023 ± 0.220	0.0
28.58	7.879 ± 0.156	7.870 ± 0.228	0.4
34.29	5.300 ± 0.180	5.311 ± 0.433	0.4

Table 3. Comparison of TRIPOLI-4® reaction rates on ^{115}In when using JEFF-3.1.1 or FIFRELIN n/γ-uncoupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-uncoupled	Rel. err. (nb. σ)
5.72	7.193 ± 0.162	6.842 ± 0.119	24.9
11.43	3.352 ± 0.155	3.202 ± 0.167	20.2
17.15	1.652 ± 0.218	1.574 ± 0.219	15.6
22.86	0.840 ± 0.265	0.805 ± 0.273	11.1
28.58	0.440 ± 0.354	0.425 ± 0.360	6.9
34.29	0.239 ± 0.435	0.231 ± 0.411	5.8

Table 4. Comparison of TRIPOLI-4® reaction rates on ^{115}In when using JEFF-3.1.1 or FIFRELIN n/γ-coupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-coupled	Rel. err. (nb. σ)
5.72	7.193 ± 0.162	7.171 ± 0.180	1.3
11.43	3.352 ± 0.155	3.347 ± 0.280	0.5
17.15	1.652 ± 0.218	1.637 ± 0.324	2.4
22.86	0.840 ± 0.265	0.839 ± 0.442	0.4
28.58	0.440 ± 0.354	0.438 ± 0.526	0.8
34.29	0.239 ± 0.435	0.237 ± 0.637	1.2

Table 5. Comparison of TRIPOLI-4® reaction rates on ^{32}S when using JEFF-3.1.1 or FIFRELIN n/γ-uncoupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-uncoupled	Rel. err. (nb. σ)
5.72	1.321 ± 0.232	1.219 ± 0.238	24.0
11.43	0.477 ± 0.352	0.440 ± 0.363	15.8
17.15	0.182 ± 0.563	0.169 ± 0.601	9.4
22.86	0.070 ± 0.804	0.066 ± 0.932	4.9
28.58	0.028 ± 1.345	0.027 ± 1.567	2.9
34.29	0.011 ± 1.892	0.010 ± 2.017	2.8

Table 6. Comparison of TRIPOLI-4® reaction rates on ^{32}S when using JEFF-3.1.1 or FIFRELIN n/γ-coupled mode.

Depth (cm)	R.Rate ± σ (%) with JEFF-3.1.1	R.Rate ± σ (%) with FIFRELIN n/γ-coupled	Rel. err. (nb. σ)
5.72	1.321 ± 0.232	1.256 ± 0.361	11.6
11.43	0.477 ± 0.352	0.455 ± 0.597	7.0
17.15	0.182 ± 0.563	0.170 ± 0.836	6.7
22.86	0.070 ± 0.804	0.067 ± 1.274	3.0
28.58	0.028 ± 1.345	0.027 ± 2.146	2.3
34.29	0.011 ± 1.892	0.010 ± 3.285	2.0

In the case of the n/γ-uncoupled mode of FIFRELIN, significant differences with JEFF-3.1.1 results are observed for all responses, particularly at the surface positions closest to the fission plate. This suggests that the spectral effect of FIFRELIN data noticed in the previous section, at the emission of fission neutrons, has still an impact on results after neutron transport to distances up to 34 centimeters.

As for the n/γ-coupled mode of FIFRELIN, Tables 2 and 4 show no difference for the first two responses: JEFF-3.1.1 and FIFRELIN results are within 3 sigma of uncertainties for ^{103}Rh and ^{115}In dosimeters. However, Table 6 shows discrepancies up to 11.6 sigma for the reaction rates on ^{32}S. When examining Figure 2 again, the prompt fission neutron spectrum of JEFF-3.1.1 is actually closer to FIFRELIN spectrum when using its n/γ-coupled mode, which can explain the lack of significant differences in Tables 2 and 4. But bigger discrepancies between JEFF-3.1.1 and n/γ-coupled mode spectra can be noticed in Figure 3 at energies higher than approximately 2 MeV, thus explaining that discrepancies can be seen on ^{32}S response only, which has the highest reaction rate threshold (1.6 MeV).

3.3 Further investigations

Further investigations were performed through specific modifications based on JEFF-3.1.1 nuclear data file, so as to better determine the origin of the differences noticed in Tables 1, 3, 5 and 6.

First, the same trend in results was observed when running TRIPOLI-4® with modified evaluated data of the prompt fission spectrum that consist in suppressing the dependence on the incident neutron energy by extending the evaluated data for thermal incident neutron energies to the whole incident energy range of the prompt ^{235}U fission spectrum. This means that the previously noticed differences are not due to the fact that FIFRELIN data, as used in this coupling work, do not depend on the incident neutron energy but are valid for a given energy range only.

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Then, in another test, when replacing the prompt fission spectrum by the average prompt neutron fission spectrum, as illustrated in Figure 2, from respectively both modes of FIFRELIN, all TRIPOLI-4® results turned out to be very close to the results obtained with TRIPOLI-4®-FIFRELIN coupling (within 3 sigma of uncertainties). This suggests that the coupling results, which take advantage of the prompt fission neutron multiplicity distribution and of energy conservation per fission event, are not directly sensitive to the difference observed in Figure 4 (which remained unchanged after these respective modifications of the evaluated data), but only to the difference of average prompt fission spectrum.

In order to clarify the contribution of the fission model, apart from the sensitivity to a difference of average spectrum, we performed an analysis based on non-average reaction rates. Full distributions were built by means of simulations containing only one neutron. For that purpose, we modified the previous configuration in order to obtain a 4π-solid angle detection: this allowed us to take into account coincidences between neutrons emitted in a same fission event. The new configuration consisted in several concentric iron spheres and reaction rates were calculated at each spherical interface. We kept the previous modification of this Subsection for the simulation using evaluated data. As an example, Figure 5 shows very different distributions of ^{103}Rh reaction rate at the first interface (at a depth of 5.72 centimeters) obtained by simulating a single neutron per batch. In this figure, FIFRELIN events were produced with the n/γ-uncoupled mode of FIFRELIN.

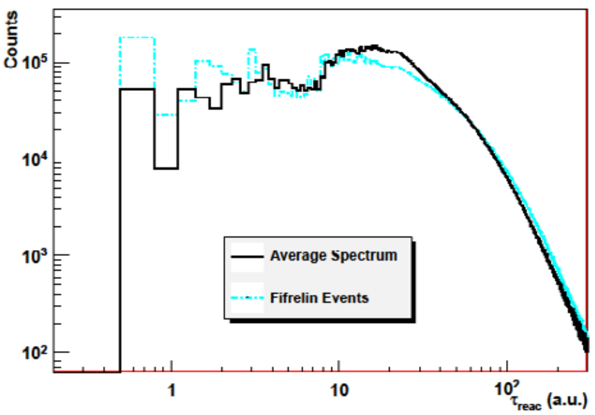

Fig. 5. Distributions of ^{103}Rh reaction rates.

In a similar way, different distributions would also be found with the n/γ-coupled mode of FIFRELIN when compared to the related average spectrum retrieved from evaluated data.

4 Conclusion

FIFRELIN fission model and TRIPOLI-4® Monte Carlo transport code have been coupled through external files, so as to simulate a detailed model of fission together with an accurate transport of the fission neutrons.

Calculations on a modified version of the ASPIS benchmark, either with JEFF-3.1.1 data or with the coupling with FIFRELIN code for the fission sampling on ^{235}U, showed significant differences on reaction rates which turned out to be mainly due to the slight difference of average prompt fission spectrum. However, the n/γ-coupled mode of FIFRELIN actually gave average reaction rates closer to those obtained with the evaluated data than its n/γ-uncoupled mode.

A complementary analysis was performed so as to clarify the real impact of the fission model after neutron transport, apart from the average trend: the distribution of reaction rates per fission event turned out to be very different with or without the use of FIFRELIN, highlighting the capability of the present coupling to take into account coincidences between neutrons emitted by a same fission event, which are still visible after neutron transport.

In a future work, other applications involving an analysis of events in coincidence could also be addressed, such as a time analysis of fission neutrons after transport.

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