THE TENDL NUCLEAR DATA LIBRARY: FOR CRITICALITY CALCULATIONS AND MORE

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ABSTRACT

Nuclear data libraries are a key component of many neutronic simulations, including criticality safety calculations. They are regularly validated with criticality safety benchmarks, eventually showing various degrees of performance, depending on the benchmark selection. The evaluations performed in the TENDL library, especially with its latest releases in 2021 and 2023, are increasingly associated with other international libraries, such as the JEFF library. There is therefore a need of an improved performance for the TENDL evaluated files, with respect to traditional criticality calculations, especially for minor actinides and fission products.
Additionally, the TENDL library covers a large range of isotopes, often going beyond the coverage of other libraries. It is consequently the default choice for users when no alternative exists, but increasingly also the choice when TENDL outperforms other libraries. Recent improvements for fission products in both the thermal and fast range have shown a positive impact on burnup calculations. A major update of all TENDL minor actinide nuclear data files is underway. As usual, emphasis will be put on reproducibility and efficiency of evaluation methods for TENDL.

KEYWORDS

TENDL, Nuclear data, evaluation, criticality

1. INTRODUCTION

The TENDL library stands for “TALYS Evaluated Nuclear Data Library”, and is released every year or second year since 2008. It is in many aspect similar to other nuclear data libraries, such as JENDL-5 [1], JEFF-3.3 [2] or ENDF/B-VIII.0 [3], and was extensively described in a number of publications, see for instance [4]. It contains nuclear data evaluations for many relevant nuclides, follows the ENDF-6 format, provide recommendations (or evaluations) from 0 eV up high energy (in a systematic manner), includes covariance information, provides sublibraries for neutrons but also for charged particles, up to incident alpha. From these aspects, it is not different to the other mentioned library projects.
There are nonetheless a number of originalities in TENDL, both in the way it is produced and in its distributed files. To start with, as its name indicates, it is based on a nuclear reaction code, TALYS [5], for all nuclides and incident particles. Naturally, TALYS does not produce all necessary quantities required for the making of an evaluation, and it is therefore complemented by other codes. But the philosophy remains the same: producing the complete nuclear data files only with codes and scripts. This leads to the second specificity of TENDL: it can be reproduced by anyone, at anytime, as the complete set of codes and input files are available on the TENDL website, or on request. Another difference worth mentioning is the availability of covariance matrices (and so-called equivalent

perturbed, or "random" files) for all nuclides. This renders the calculation of uncertainties for any application, which depends on nuclear data, possible.
Such aspects can be of tremendous importance for applications related to criticality-safety. By using TENDL, or combining it with other libraries, users have the possibility to make every nuclide reacting, as cross sections become available (for instance in the ACE format for Monte Carlo simulations). They can also calculate uncertainties virtually due to all nuclides, as covariance matrices (or random files) are also systematically available. These two features are naturally of prime importance in criticality-safety and contribute to the application of approaches such as best estimate plus uncertainties (BEPU) or burnup credit (BUC).
In the following, the aspects of interest for criticality-safety applications are presented, as well as other characteristics, naturally linked to the TENDL principles: unicity, reproducibility, completeness, and quality.

2. THE TENDL PHILOSOPHY

Since the first release of the library, the TENDL philosophy has not changed: allowing any evaluation to be reproduced (no manual intervention and storage of all adjusted parameters), applying this principle to all nuclides living longer than 1 second, being complete, and finally improving the nuclear data quality by using adequate parametrization. A number of codes are used for the production of evaluated files, as indicated in Fig.1.

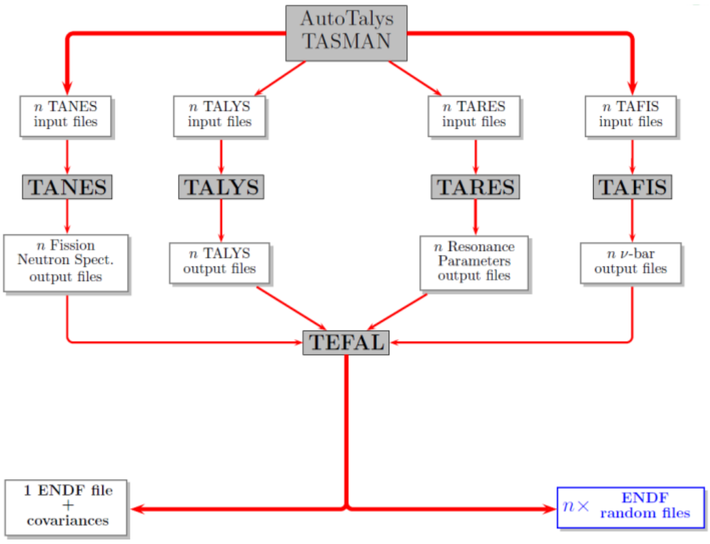

Figure 1. Codes and scripts used to produce the TENDL library.

TALYS remains the main code, producing cross sections and differential spectra. In the case of neutron-induced reactions, it is complemented by other codes, such as TARES (for the resonance parameters), TANES (for the neutron fission spectra), TAFIS (for the average neutron emission in fission), TEFAL (for the ENDF-6 formatting) and finally TASMAN (for the generation of perturbed model parameters). The application of these codes to all nuclides is performed with a simple Shell script, called Autotalys. The outcomes of this code structure are ENDF-6 formatted files, with covariances, or equivalent perturbed ENDF-6 files, as well as a number of processed files for specific codes.
For nuclides with experimental data, the parameters of the above codes can be adjusted to obtain a good agreement between calculated and experimental nuclear data. Once such selection of parameter values is performed, the optimal parameters are stored in dedicated directories, to be used for subsequent TENDL versions. In the last release of the library, especially thanks to the strong link with the JEFF library, efforts were applied in improving fission products (*e.g.* Eu, Sm, Pm, Rh, Cs), with a dedicated focus in the resonance range. Cases of importance in reactor physics were improved by importing high-quality resonance parameters from JEFF or from the n_TOF facility. To illustrate the improvement, Fig.2 is showing the case of ^{105}Rh, where the resonance range has been modified to be better in agreement with expectations from reactor physics.

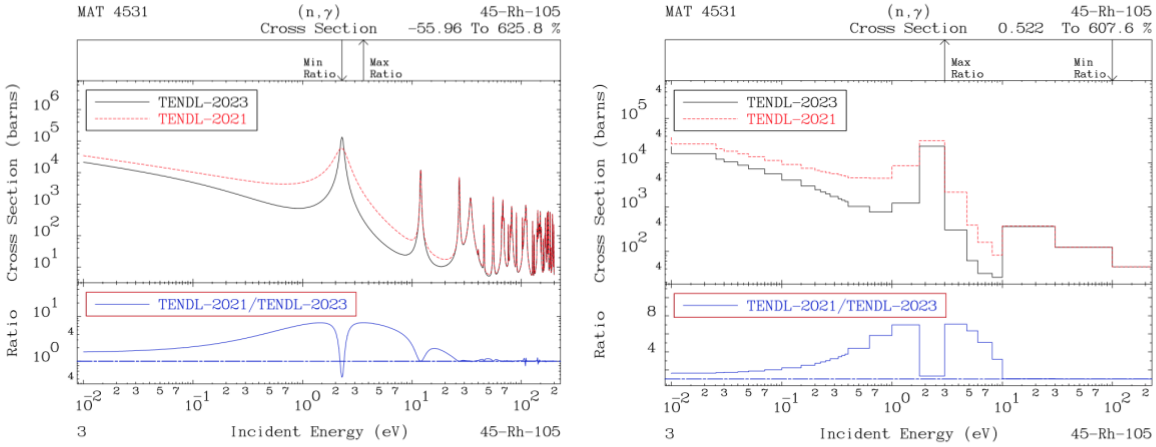

Figure 2. Example of improvement for the capture cross section on ^{105}Rh; left: pointwise cross section, right: groupwise cross section.

Similarly, the covariance matrices for a number of minor actinides were also improved, as a collaborative work with the JEFF community. In the case of ^{236}U, the evaluation of the JEFF-3.3 library did not contain covariance information; in order to correct this deficiency for the next release of the JEFF library, the covariance matrices from the TENDL-2023 evaluation are included in the future JEFF file.

As TENDL contains more than 2800 nuclides, many cases are to be calculated without experimental data. This is performed by applying systematics of model parameters, in the fast neutron range (above the resonance range), as well as down to the thermal range (applying the HFR approach [6,7]).
A number of methods have been developed since the first TENDL release, expanding the original philosophy to some application fields. It is worth mentioning specific applications in astrophysics with the calculations of various quantities of relevance (such as the Maxwellian Averaged Cross Section, or MACS), available in TENDL-2021 and TENDL-2023. In this case, the ENDF-6 format is not necessary, and output files are provided in simple text format, for more than 8000 nuclides, with model uncertainties. Another application of the TENDL method is in the field of uncertainty propagation, with the development of the Total Monte Carlo (or TMC) method [8,9] and the Bayesian Monte Carlo (or BMC) method [10,11].
As a final general comment on the TENDL library, its nuclear data evaluated files have been included in a number of general-purpose libraries, such as JEFF-3.3 and ENDF/B-VIII.0, but also in fusion and activation related libraries [12,13]; codes for specific applications have recently included TENDL evaluations in their processed libraries, such as FISPACT [14], CASMO5 [15], GEANT [16] and FLUKA [17].

3. APPLICATIONS FOR CRITICALITY SAFETY

In the field of criticality-safety, the TENDL library, eventually complementing other libraries or used on its own, can be of an added value for the two mentioned reasons: completeness and uncertainties. These two specific subjects are detailed below.

3.1. Criticality benchmarks

Nuclear data libraries are often validated using criticality-safety benchmarks. Such validation is in general limited to k_{eff} values and to much less extend to reaction rates. Examples of TENDL validations, together with other libraries, can be found in [18]-[20]. For the last few versions of the TENDL library, systematic validations with criticality benchmarks are performed. Such type of studies can be performed on a large scale (for all, or almost all, available criticality benchmarks), or for targeted cases in order to study the effect of a specific nuclide evaluation. For a statistical study with a large number of benchmark cases, an example is presented in Fig.3 for thermal plutonium solutions.

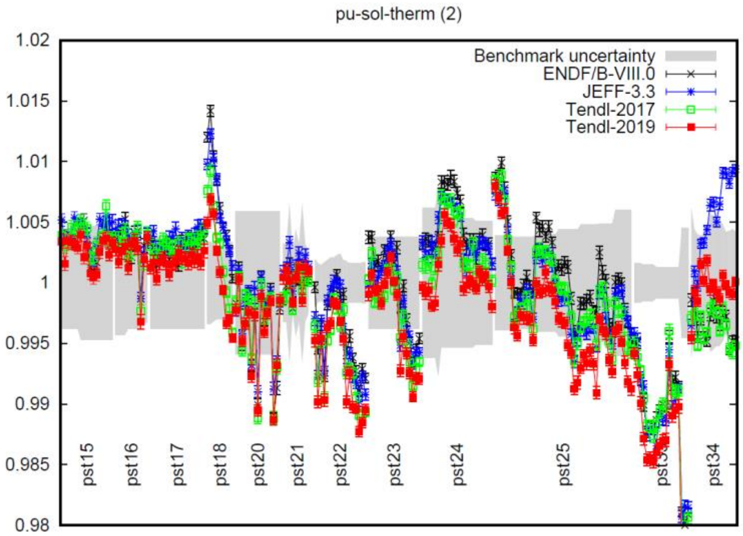

Figure 3. Example of the validation of the TENDL library for a large number of benchmarks.

If it is difficult to extract information on a specific case with this example of study, it can help in finding trends, for instance as a function of a nuclide, its concentration, or its location in the fuel or in the reflector. This can indicate if an evaluation contains adequate cross sections or angular distributions. Naturally, this process allows to validate a limited number of the TENDL evaluations, but nonetheless for the most relevant nuclides in criticality-safety (for fresh fuel). In the case of a targeted study, an example is presented in Figs.4 and 5.

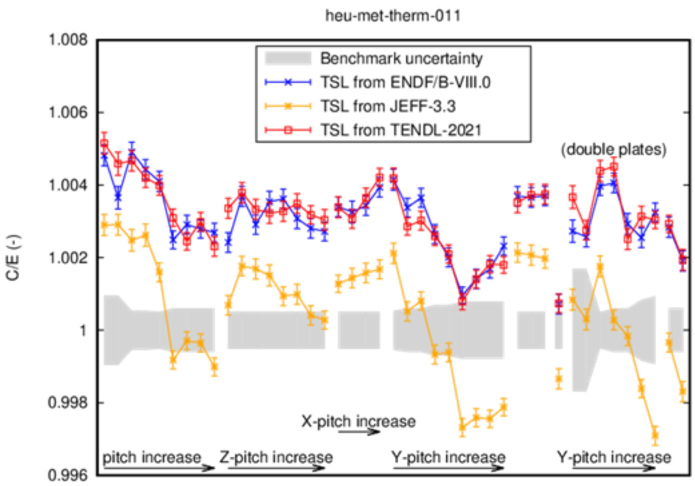

Figure 4. Example of a targeted validation of the TENDL library (with a specific benchmark), with different thermal scattering data.

In Fig.4, the validation of the TENDL-2021 library was performed with the criticality benchmark called HEU-MET-THERM-011, for a metallic highly ^{235}U enriched system, with a thermal neutron spectrum. As observed, the impact of the thermal scattering data (or TSL) is important, and this study indicated that the TSL from the JEFF-3.3 library, in combination with the TENDL-2021 evaluated files lead to the best agreement with the benchmark values.

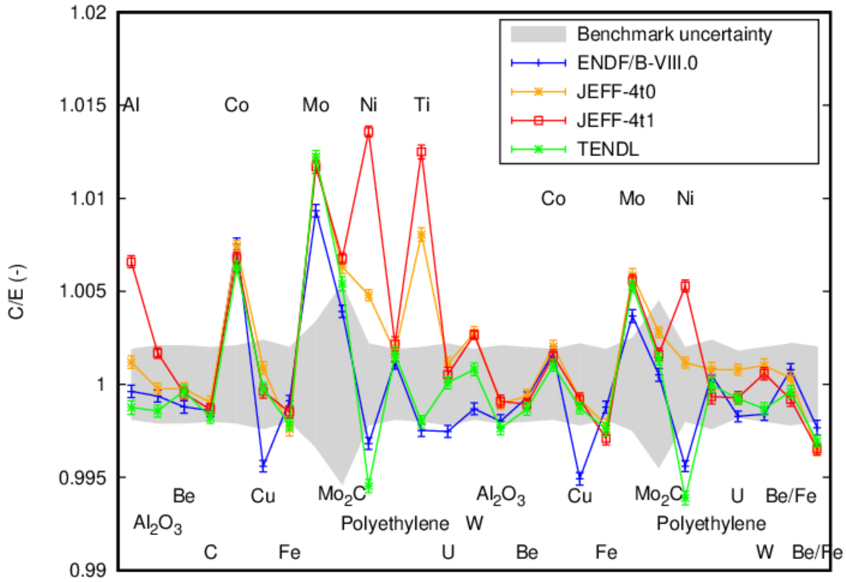

Figure 5. Example of a targeted validation of the TENDL library with the HMF84 benchmarks sensitive to specific nuclides.

In Fig.5, different cases of the HEU-MET-FAST-084 criticality benchmark are first selected as a function of their sensitivities to specific nuclides. In this example, structural materials are for instance indicated. By comparing the ratios of the C/E (Calculated over Experiment) values, one can deduce the impact of a specific evaluation. Such steps are performed with various independent evaluated files.
This process is not specific to the TENDL library for criticality benchmarks, but in the case of TENDL, such validation is combined with other quantities of interest, such as the degree of agreement with activation benchmarks, fusion benchmarks, or with the agreement with the EXFOR database for thermal cross sections, capture integrals or MACS [21]. This allows to eventually focus less on criticality benchmarks, and therefore to have a library less targeted towards k_{eff} from criticality benchmarks and being more of a general-purpose perspective.

3.2. Uncertainties

The calculation of uncertainties is also an important aspect in criticality-safety studies, particularly in BEPU and BUC [22]. Nuclear data is one of the main contributors to such uncertainties, and TENDL evaluations, systematically containing covariance information, can bring a complementary and complete answer.
Traditional methods such as first-order perturbation and linear approximation can be used [23]-[24], but also less approximative approaches such as TMC are easily applicable based on perturbed files from the TENDL website (the JEFF project is also providing such files). In some cases, only TMC or TMC-like methods can be applied (for instance with thermal scattering data, fission yields, of transient calculations [25]-[26]). Comparisons between first-order perturbations and TMC were performed for a large number of benchmarks, showing that TMC generally leads to larger uncertainties [27]. One of the reasons for differences between the covariance-based method and with perturbed nuclear data files is related to the approximation of normality, inherent to the covariance matrix, where a probability density function (pdf) is approximated by a normal distribution. This is justified in cases where uncertainties (standard deviations) are not too large. An example is presented in Fig. 6.

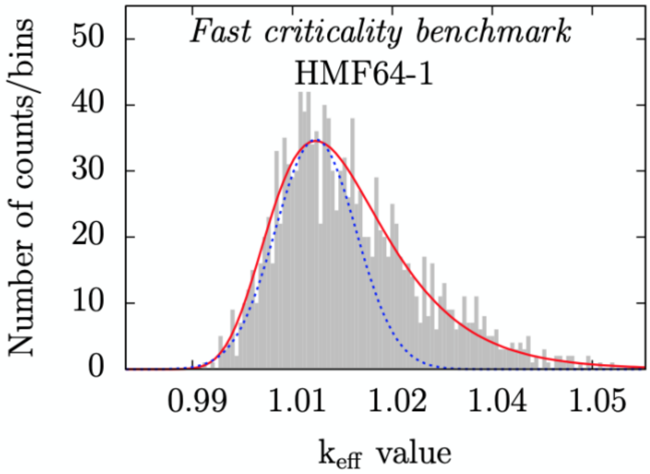

Figure 6. Example of uncertainties due to nuclear data for the HMF64, case 1 benchmark, using perturbed nuclear data files for uncertainty propagation.

In this example for a metallic ^{235}U highly enriched benchmark with a fast neutron spectrum, the uncertainties due to nuclear data, obtained with perturbed files (TMC method) is larger than in the case of the approximation of normality (blue curve). There is a large tail of cases for high k_{eff} values, increasing the uncertainties, but also strongly changing the confidence intervals. The origin of such difference comes from the fact that this benchmark is sensitive to the ^{208}Pb cross sections, which are not represented by a normal pdf.

Depending on the studied cases, TENDL can lead to valuable information for criticality uncertainties, complementary to other library projects, by exploring non-linear effects and by systematically providing uncertainties due to all nuclides.

4. CONCLUSION

The TENDL library, being released since 2008, has proven to be useful for a vast range of applications, including criticality safety. The advantages are at least two folds: completeness (all relevant nuclides are provided with best-estimate nuclear data and uncertainties) and the possibility to assess non-linear effects. The joining of effort between the TENDL group and other library projects is beneficial for the criticality safety user community, globally improving evaluations for relevant nuclides. It is expected that the quality of TENDL will continue to improve, finally reaching the high quality standards set up by other library efforts.

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