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TENDL-2011: TALYS-based Evaluated Nuclear Data Library

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ABSTRACT

The 4^{th} release of the TENDL library, TENDL-2011 (TALYS-based Evaluated Nuclear Data Library) is described. This library consists of a complete set of nuclear reaction data for incident neutrons, photons, protons, deuterons, tritons, helions and alpha particles, from 10^{-5} eV up to 200 MeV, for all isotopes from ^{6}Li to ^{281}Ds that are either stable of have a half-life longer than 1 second. All data are completely and consistently evaluated using a software system consisting of the TALYS-1.2 nuclear reaction code, and other programs to handle resonance data, experimental data, data from existing evaluations, and to provide the final ENDF-6 formatting. The result is a nuclear data library with mutually consistent reaction information for all isotopes and a quality that increases with yearly updates. To produce this library, TALYS input parameters are adjusted for many nuclides so that calculated cross sections agree with experimental data, while for important nuclides experimental data are directly included. All information is available on www.talys.eu and www.talys.eu/tendl-2011.

Key Words: nuclear data, covariances, TALYS

1. Introduction

During the 1980's, nuclear model codes like STAPRE, GNASH and EMPIRE became available. The procedure for producing an evaluated library was the following: perform an evaluation of experimental data, and complement this with nuclear-model based predictions for important channels and energy ranges for which no experimental data are available. In the last decade, nuclear data libraries have become more complete in coverage of reaction channels, thanks to nuclear model codes, and are now also more often accompanied by uncertainty data.

The strategy behind the TENDL library is different: Largely based on the TALYS nuclear model code, to produce a based nuclear data library for *all* nuclides and projectiles, complete in reaction channels, secondary distributions, and covariance data, and *overrule* these model-based data by experimental data for nuclide-channel-energy combinations for which TALYS can not deliver the required quality on its own. This leads to a much more consistent set of nuclear data libraries, since one isotopic evaluated file differs from the next one only with regards to the availability, and hence the influence, of more or less experimental information, while all isotopic evaluations are equally complete, consistent and processable.

The TENDL library is only one spin-off of a new method of nuclear data evaluation and validation, which revolves completely around *reproducibility*: only the most essential components of an evaluation should be used and stored for future use: selected experimental data sets, a TALYS input file with adjusted parameters, and possible additional scripts for e.g. adoption of

data from existing libraries. In fact, this collection of ingredients form the “data evaluation”, not the ENDF-6 formatted data library. Sticking to this “rule” opens unprecedented possibilities. For example, it can easily be imagined that if nuclear data library production is so well automated, that it is easy to produce hundreds or thousands of random ENDF files for the same isotope by perturbing nuclear model and resonance parameters, enabling exact and (equally important) easy propagation of nuclear data uncertainties. This can even be taken a step further [1] by automatically optimizing nuclear data libraries, through e.g. minimizing the total C/E of k-eff values for many benchmarks, and adopting the optimal random library. Some of these may find their way into TENDL. Finally, the reproducibility condition allows nuclear data libraries to be easily reproduced when better ingredients become available, or when e.g. shortcomings in TALYS are repaired. As long as the evaluation input files per isotope are kept, this will lead to libraries with progressively increasing quality.
Nuclear data evaluation can thus be performed much more efficiently and one result is the TENDL library. We basically focus on three aspects of nuclear data libraries that we find equally important:

1. Realistic central values. In the early days of nuclear science this was, necessarily, the only issue under attention, since conditions 2. and 3. below could not yet be fulfilled. It still holds as the prime concern today: High-quality experimental data, complemented by powerful nuclear models, should be used to simulate reality as close as possible. Often there is a trade-off between differential and integral performance, while ideally these are excellent simultaneously.
2. Covariance data. Nuclear data uncertainty information and its propagation through applied reactor software is essential for an adequate safety and economy analysis of a nuclear device. The intrinsic quality of the central values mentioned under 1. is reflected by covariance data.
3. Completeness of the nuclear reaction description. This ensures that no phenomenon is neglected altogether in applied calculations. Important examples of omissions are unrealistic isotropy by leaving out angular distributions, incorrect gamma heating due to the absence of photon production data, etc. Omission of an entire class of secondary reaction information means also that the propagated effects of nuclear data uncertainties are underestimated.

Table I is an attempt to classify all nuclides in groups of importance, “summed over applications”. This classification is based on experience, amount of literature, data user requests, etc. The list applies to fission, fusion and accelerator (such as medical) applications, although fusion and accelerator scientists would probably leave out the actinides from this list, and each of the three communities is generally interested in a different energy range (which is left out of Table I for simplicity). For the Nuclear model column of Table I, the situation is different. In principle, complete nuclear model calculations can be performed for *all* nuclides, reaction channels and energies, important or not. In fact, the basis for TENDL is formed by complete nuclear data libraries, all with essentially the same structure, for all material categories (1) to (12). The first version of the library, TENDL-2008, was just that: the isotopic nuclear data libraries were made by global TALYS calculations, without any further adjustment of any model parameters or inclusion of experimental data. In more recent versions of TENDL, progressively more effort is invested in nuclide specific parameters and experimental data as we move up the list from category (12) to (1), until for the most important channels, e.g. ^{238}U(n,γ), nuclear model calculations are completely normalized by experimental data, or differential data inferred from integral measurements, in certain energy ranges. In sum, TENDL-2011 contains all cases present in Table I, i.e. it ranges from detailed evaluation work to completely ”blind” libraries. This new approach should not be confused with “quick and dirty” or “blind automated” nuclear data production, it should rather be called “systematic evaluation”. What this approach guarantees is that all information emerging from large efforts invested in single nuclide evaluation will remain at our disposal forever: reproducibility of the evaluation process is essential, while a bare undocumented ENDF-6 file, produced by a retired evaluator, usually does not give a lot of insight.

2. Methodology

The working method to produce the TENDL library has already been presented in a few dedicated papers (see for instance Refs. [2–5]). It is not specific to actinides, although it should be mentioned that the main difference between an evaluation of a major actinide and a regular isotope is the amount of time spent to obtain the best possible TALYS input parameters. As mentioned before, once these input parameters are known (together with their uncertainties), they are stored to be re-used as needed. The complete schematic approach is presented in Fig. 1.

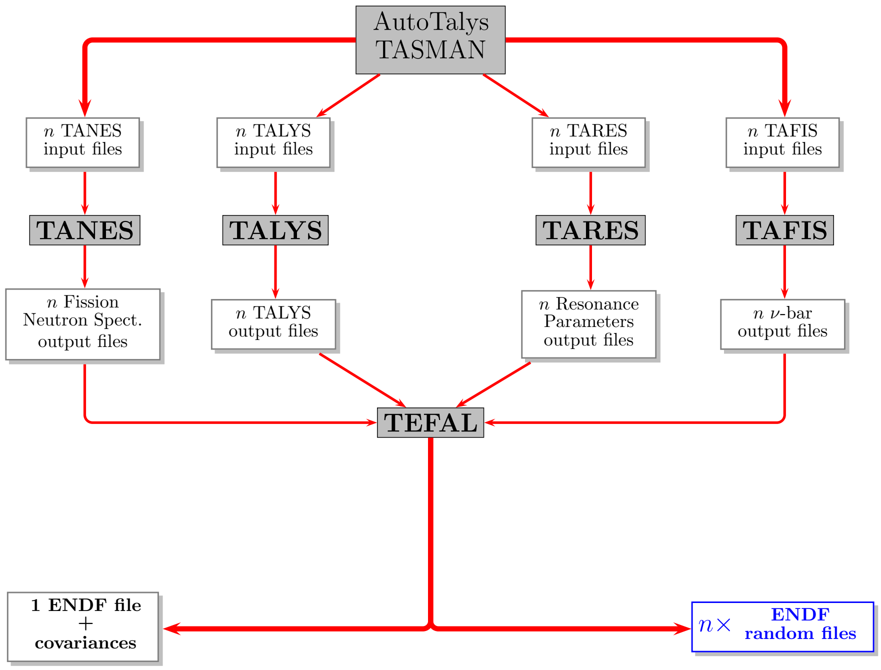

Figure 1. Flowchart of the nuclear data file evaluation and production with the TALYS system.

The full nuclear data library production relies on a small number of codes and programs, automatically linked together. The output of this system is either one ENDF-6 formatted file, including covariances if needed, or a large number of random ENDF-6 files for the TMC method. For TENDL, the best possible single ENDF-6 file is included. The central evaluation tool is the TALYS nuclear model code. A few other satellite programs are used to complete missing information and to provide uncertainty information. At the end of the calculation scheme, the

Material	Experimental data	Nuclear models	Evaluation/Validation
(1) The Big Three: ^{235,238}U,^{239}Pu	High-quality measurements (<2 % for important channels), directly (cor)related with neutron standards More than 10-20 exp. data sets in same energy range	Models overruled by experimental data for important channels: complete normalization of model results	Need for reliable experiment-based covariance data Direct feedback from integral measurements: criticality, reactor systems, inventory, etc.
(2) Important coolants and structural materials: H, C, O, Fe	Many experimental data sets for many channels uncertainty $<10\%$ (dosimetry reactions <3 %)	Precise nuclear model calculations with many parameters to interpolate between measurements	Sometimes differential data overruled by data with better integral performance
(3) Other coolants and structural materials: N, Na, Al, Si, Ti, V, Cr, Mn, Ni, Cu, Zr, Mo, W, Pb, Bi,...		Parameter adjustment for well-measured channels	
(4) Other important actinides: ^{232}Th,^{233}U,$^{240-242}$Pu	Many experimental data sets for only the most important channels	Models used for almost all secondary distributions (angles, spectra, photons, etc.)	Isolated benchmarks available for transport or activation analyses
(5) Important fission products: ^{99}Tc, ^{103}Rh, ^{129}I,....			
(6) Breeding materials and reflectors: Li, Be,...		Model calculations with a few parameters adjusted to the few exp. data sets	
(7) Absorbers: Gd, Hf,...			
(8) Minor actinides: ^{241,242m,243}Am,^{237}Np,....	Experimental data only available for (low energy) total, elastic, capture (resonance parameters) and a few other channels		Global covariance estimates
(9) Remaining materials (natural isotopes): P, S, Cl, Ca,....			Automatic production of data libraries
(10) Remaining long-lived nuclides ($\tau>1$ year)			
(11) Medium long-lived nuclides (1000 sec. ¡ $\tau<1$ year)	(Almost) no experimental data	Complete reliance on nuclear models, preferably microscopic	(Almost) no integral experimental data
(12) Short-lived nuclides ($\tau<1000$ sec.)			Astrophysics

Table I. Classes of materials and related evaluation aspects, in decreasing order of technological importance.

formatting code TEFAL produces the ENDF files.

- The nuclear reaction code TALYS has been extensively described in many publications, see e.g. Refs. [6,7] and is now widely used for basic physics and nuclear applications, see the first 315 references of the bibliography of Ref. [6]. It simulates reactions that involve neutrons, gamma-rays, *etc* from thermal energies up to 200 MeV.
- TASMAN is a computer code for the production of uncertainty data using results of the nuclear model code TALYS, and for automatic optimization of the TALYS results with respect to experimental data (parameter fitting).
- TEFAL is a computer code for the translation of the nuclear reaction results of TALYS, and data from other sources if TALYS is not adequate, into ENDF-6 formatted nuclear data libraries.
- TARES is a code to generate resonance information in the ENDF-6 format, including covariance information.
- TANES is a simple program to calculate the fission neutron spectrum based on the Los Alamos model [8].
- TAFIS is used to calculate fission yields, prompt neutron emission from fission and other necessary fission quantities.
- Autotalys is a shell script which takes care of the communication between all software described above and runs the complete sequence of codes for a user-specified configuration.

3. The TENDL-2011 library

The TENDL-2011 library contains eight sub-libraries for incident neutrons, protons, deuterons, tritons, helium-3, alphas, photons and fission yields. As described in the following sections, different types of files are included in the sublibraries. Three types of formatted files, different tabulated and processed files are provided:

- ENDF files: formatted in the ENDF-6 format, up to 200 MeV for isotopes with half-life longer than 1 sec, containing sections MF1 to 15 and MF-30 to 35. A pointwise version, called PENDF, is also provided,
- EAF files: formatted following European activation files up to 60 MeV, containing sections MF3 and MF33,
- Activation files: up to 200 MeV for isotopes with half-life longer than 1 year, 60 MeV otherwise, containing sections MF3, 6 and 33,
- Tabulated files for partial, residual cross sections, gamma-ray intensities and angular distributions,
- Processed ACE files at room temperature and covariances (tabular and plots).

3.1. Neutron sublibrary

For incident neutrons, nuclear data libraries for 2375 isotopic targets are produced. These are all isotopes, in either ground or metastable state, with a half-life longer than 1 sec. from $Z = 3$ (Li) to $Z = 110$ (Ds). All libraries extend up to 200 MeV. As explained in the introduction, one consistent production method for these nuclear data libraries was used, and they are all complete in terms of reaction information. However, in line with Table I, progressively more effort was invested when moving from the exotic nuclides to the most important nuclides. Hence,

1. For more important nuclides, more TALYS parameter adjustment and inclusion of experimental data takes place. Also more and better resonance information is generally available.

2. For more important nuclides, a larger number of random TALYS runs to construct a covariance matrix was used. This number ranges from 3 random runs for the most exotic nuclides to several hundred for the most important ones. Here, it suffices to state that more random runs leads to a more statistically converged covariance matrix.

For each isotope, tabular outputs of TALYS are presented in different sub-directories for cross sections, angular distributions, gamma-ray emission and spectra. They allow for easy plotting against experimental data. Also the used input files are stored. Important for applied calculations are the ENDF-6 formatted files and the processed nuclear data libraries. Various different (in terms of ENDF-6 procedure) versions of an isotopic evaluation are available, as well as a variety of processed libraries for both central values and covariance data.

A typical data file contains the following sections:

- MF-1: General information and fission parameters (average number of prompt, delayed and total fission neutrons, and fission energy release),
- MF-2: Resonance parameters (in Reich-Moore or Multi-level Breit-Wigner format),
- MF-3: Cross sections (total, elastic, inelastic, capture, (n,2n), fission, and others),
- MF-4: Angular distributions,
- MF-5: Fission neutron spectrum,
- MF-6: Double differential spectra, photon production, residual production cross sections and recoils,
- MF-8-10: Isomeric cross sections,
- MF-12-15: Gamma yields, angular distributions and spectra,
- MF-31-32-33-34-35: Covariance data for average number of fission neutrons, resonance parameters, cross sections, angular distributions and fission neutron spectra.

3.1.1. Resonance range

The resonance range is represented in terms of resonance parameters following either Reich-Moore (for the vast majority of cases) or Multi-level Breit-Wigner formalism (for actinides). The resonance range is produced with the TARES code using known resonance parameters from compilations or existing evaluations. If resonances are not known for short-lived nuclei, a simple approach is used to produce fake resonances, as explained in Ref. [9].
For the unresolved resonance range, known parameters are obtained from existing evaluations. The parameters are then randomized to produce covariance files and random ENDF files.

Resonance parameters are extracted from the latest measurements (such as from the EXFOR database [10]), and from compilations (*i.e.* The Atlas of Neutron Resonances [11]). These two sources of information cover the vast majority of experimental data used for the isotopes in TENDL. Alternatively, for major actinides and other important structural materials, resonance parameters are imported from existing evaluations. As often uncertainties are not included in other libraries, resonance parameter uncertainties are then obtained from other sources (such as EXFOR).
For the remaining ones, hypothetical resonance levels are used with a bound level to simulate the elastic, capture and fission cross sections below several keV. The parameters of these resonances are extracted from average level spacings D_0, $s-$wave strength functions S_0, radiative widths Γ_γ and scattering radius calculated with TALYS.
An original unresolved resonance range (URR) is now included for all isotopes of TENDL-2011, based on TALYS parameters.

3.1.2. Fast neutron range

Cross sections in the fast neutron range and differential data are obtained from the TALYS-1.2 nuclear reaction code. It simulates reactions in the keV-200 MeV energy range for target nuclides of mass 12 and heavier. The quality of the evaluations in the fast neutron range can be classified in three categories, depending on the amount of ”knowledge” (*e.g.* experimental data) which is included in the calculation scheme.
For the vast majority of unstable nuclei except the actinides, in the absence of experimental information, default TALYS calculations were performed to obtain cross sections, angular distributions and differential data. These results were directly formatted to the ENDF-6 format. Default model parameters were then applied, which follows systematics globally adjusted for stable isotopes.
For stable isotopes, actinides and long-lived nuclei for which experimental data are available, adjusted TALYS parameters were used to reproduce experimental information.
In the case of some particularly important isotopes (such as ^{235}U or ^{238}U), an extra step in the evaluation procedure is made, applying minor adjustments to cross sections to obtain good $\mathrm{k}_{\mathrm{eff}}$ benchmark results.

3.1.3. Covariance information

The methods as presented in Refs. [2,12] are used to generate covariances. Three types of covariance information are stored in our evaluations.

From thermal energy to the end of the resonance region, covariance information is stored in the compact MF-32 format (resonance parameter covariances), as defined in Ref. [13]. Resonance parameter uncertainties (resonance energy and elastic, radiative and fission widths) are obtained from the same source as resonance parameters when possible, ensuring consistency. If no uncertainties are given in literature, default values of 0.1 % and 50 % are assumed for resonance energy and widths, respectively. Short-range correlations are calculated as presented in Ref. [12]. No long-range correlations are used.
In the fast neutron range, we use a Monte Carlo method in which the covariance data come from uncertainties of the nuclear model calculations. For all isotopes, the initial "best" set of results is produced by a TALYS, TAFIS or TANES calculation with an adjusted input parameter set. This set of results is stored in file MF-1 to MF-10. Next, for each isotope we have performed runs with random nuclear model parameters, which are used to generate uncertainties and correlations. Besides correlation within the same reaction channels, also correlation between reaction channels is included. All information on cross section, nubar, fission neutron spectrum and angular distribution covariances are stored in the MF-30, 31, 33 and 35 format, starting at the end of the resonance range up to 20 MeV.

3.2. Other sublibraries

3.2.1. Proton sublibrary

Complete proton data libraries for about 2400 isotopes, i.e. all isotopes with half life longer than 1 seconds, with energies from 1 to 200 MeV have been produced. All calculations are performed with default parameters, even though we are well aware that better fits to experimental data can be obtained for several nuclides. The proton data libraries are thus simply an alternative to the intranuclear cascade codes used at high energies, in which also no adjustment to experimental data takes place. As the evaluation effort is relatively simpler than for neutrons, we expect to be able to zoom in on experimental proton-induced data in the coming years for all materials, like we did for incident neutrons. We note that it is our experience that the difference between a global and a parameter-adjusted evaluation is larger for neutrons than for protons, i.e. for protons there is less to be gained, and libraries produced by default TALYS calculations already perform reasonably well. In our evaluations, the structure of an ENDF-6 file for protons is as follows:
-MF1: General information.
-MF3: Reaction cross sections.
The nuclear and the Coulomb-nuclear interference cross section in MT2 is obtained by integrating the associated angular distributions. The only other section in MF3 is MT5, which contains the total non-elastic cross section, which is to be combined with the the information of MF6/MT5 to obtain particle production cross sections and (double-)differential cross sections, similar to neutrons.
-MF6: Product energy-angle distributions. First, in MT2 the relative angular distributions for the nuclear and Coulomb-nuclear interference terms of elastic scattering are tabulated on an angular grid. Next, in MT5 the production yields of particles and residual products are stored, but contrary to neutrons now for all energies, i.e. not only above 20 MeV.

3.2.2. Photon, deuteron, triton, helion and alpha sublibraries

Also for composite particles, a total number of 2400 isotopes nuclear data libraries are produced, namely for all isotopes which are stable or have a half-life longer than 1 second. The structure of the ENDF-6 data library is basically the same as for protons, i.e.: Coulomb-corrected elastic cross section (MF-3, MT-2), total nonelastic cross sections (MF-3, MT-5), Coulomb-corrected angular distributions for elastic scattering (MF-6, MT-2), and residual production cross sections, photon production and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5). As for the other sublibraries, results for total, partial and residual cross sections and spectra are stored in x-y tables.

3.2.3. Fission yields sublibraries

Independent and cumulative fission yields are provided for a large number of actinides, incident particle energies (and for spontaneous fission) and incident particles. Files from Ra to Fm are included in TENDL-2011 for incident energies from 0.0253 eV to 14 MeV. The underlying approach is as follows. All independent and cumulative fission yields are calculated with the A. Wahl systematics [14]. If a fission yield is already evaluated in another library, the evaluated fission yield is imported if larger than 0.001 %. In the case of independent fission yields, the whole distribution is renormalized to 2. In this manner, previously evaluated quantities are conserved and missing information are added from mass $A = 60$ to $A = 180$.

3.3. Formatting and Processing

The data files are created automatically using our ENDF-6 format generator TEFAL, which merges all results into a single ENDF-6 file. Each file is tested for format errors with the latest version of the CHECKR, FIZCON and PSYCHE checking codes [15]. The TENDL-2011 library was processed with NJOY-99.364 and with PREPRO-2010. Results of the processing are also presented with the library in the form of plots of cross sections, angular distributions, and tables for different energy groups. ACE files have been included for all particles at room temperature. Each file has been tested with simple MCNP runs to verify that there is no format error.

4. Discussion and Conclusion

We hope to have made clear that we now take a more modern approach towards nuclear data evaluation. A library is not made at a certain moment in time for one isotope, or for all isotopes of an element, but rather for the whole nuclide chart at once, whereby all specific evaluation info per nuclide is kept from a previous version, or updated. We expect a large step in efficiency and quality with this approach. A few observations:

1. This is currently the only existing large scale nuclear data library for transport calculations created with one consistent approach. The number of data libraries with complete covariance data is unprecedented and allows for large scale testing of covariance data in applied calculations.

2. For TENDL-2011, the evaluations for all isotopes are mutually consistent in terms of completeness, global quality and formatting.

3. An evaluation for an isotope now contains a set of resonance parameters and uncertainties, a set of TALYS input parameters and uncertainties, and in some cases a script-based set of “manual” actions such as direct inclusion of experimental data, normalization or data adoption from existing libraries. From this compact set of information the data library is generated, i.e. the ENDF-formatted data library can no longer be the starting point, but rather an intermediate product, since then all flexibility and incremental quality improvement would be lost.

4. Since TENDL-2008, the quality of the format, the central value data points and the covariance matrices has improved through adjustment of TALYS input parameters per individual nuclide. Hence, we would qualify the covariance data as ”reasonable” but not yet as ”good”. With the current systematic approach the effort to make the step from ”reasonable” to ”good” is however minimized as much as possible. Months of effort could possibly be invested in the proper evaluation of one nuclide, this does not necessarily change from the 20^{th} century approach. The central issue in our approach is however that after such a large single-nuclide effort the evaluation remains completely reproducible, and that the data library can be regenerated whenever one wants, also after newer updates or corrections.

5. The statement in item 4. also entails that the current library release also throws our defense wide open: it will certainly be possible to find examples where our data file is not yet in agreement with experimental data and performs worse than existing evaluations. Also, our uncertainties may be too large or too small. We will try to transfer such negative feedback into an upgraded version for the isotopic evaluation under consideration in the next release.

6. Even though we are not aware of it now, some specific ENDF-6 procedure may turn out not to be adequate in our library, e.g. a wrong or less favorable choice to store the data in a specific MF/MT combination with a certain procedure, leading to unexpected processing problems. If this is the case, it is probably inadequate in all our data files. Of course, it will then also be corrected in all evaluations simultaneously, when we run the next batch.

7. It is trivial to extend the number of isotopes for which full blown evaluations are produced even further. Only more computer power is required. Realistic physics for such exotic isotopes is of course another issue.

8. To enable an honest comparison with the exact uncertainty propagation method of Ref. [2] (now called “Total Monte Carlo”) we have included extensive covariance information: cross-reaction correlations are taken into account as well as angular distribution covariances.

9. If nuclear science is ever ready for a change of nuclear data format, then it should probably go through the route outlined here: since the ENDF-6 data file is no longer considered as the most basic starting point, but rather as a helpful intermediate product that can be processed for further use, it is at the level of processing the TALYS results or resonance data that a different choice for the format could be made, instead of translating a mutually inconsistent set of ENDF files from different eras.

10. For charged particles, the TENDL collection consists of data libraries for all incident light charged particles. At the moment, no generally available computer code, including MCNPX,

is able to use nuclear data libraries other than photons, neutrons and protons, although the MCNPX based MCUNED code has recently been extended to accomplish this.

11. A next target is to obtain complete flexibility regarding the adoption of other parts from other data libraries. If this has been accomplished, it would be possible to reproduce an existing library, and to complement it with data which are missing in that library (e.g. covariance data, high energy data, gamma production, etc.)
12. We will also work towards automatic optimization to integral measurements. This paper shows that it is now rather easy to validate a new library against a large collection of benchmarks, as also presented in Refs. [1,16]. The presence of both differential and integral uncertainty data allows to improve the integral performance of TENDL using sensitivity tools.

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