Nuclear Data for Basic Science and Applications

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Abstract. Reliable and up-to-date nuclear data are important for basic science and applications. The process of compiling, evaluating, validating and disseminating nuclear data will be presented in the context of two international cooperation projects coordinated by the IAEA.

1. Introduction
Nuclear data are essential for many applications in the fields of energy, medicine, environmental monitoring, and cultural heritage. Reliable, up-to-date and organised nuclear data libraries are also indispensable for nuclear physics researchers, who need the data to improve their knowledge from existing studies and to plan future activities that may lead to new discoveries.

The collection, evaluation and dissemination of nuclear data is an arduous task that relies on contributions from experts in basic and applied sciences from all over the world. Efforts on a national and international level are coordinated by international organizations such as the International Atomic Energy Agency in Vienna (IAEA) and the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development (NEA-OECD) in Paris. The development, maintenance and dissemination of nuclear data libraries is the main goal of the international networks associated with these agencies: the Nuclear Structure and Decay Data evaluators (NSDD/IAEA) [1], the Nuclear Reaction Data Centres Network (NRDC/IAEA) [2], and the Working Party on International Nuclear Data Evaluation Co-operation (WPEC/NEA) [3]. Apart from the general purpose nuclear data libraries maintained by the international networks, more specialized and targeted databases and files are developed, updated or expanded through short-term international collaborative projects that are coordinated by the two international organizations mentioned, namely the Coordinated Research Projects (CRPs) of the IAEA and the WPEC Sub-groups of NEA-OECD.

In this paper we present a summary of the scope and outputs of two internationally coordinated research projects of the IAEA, one focusing on beta-delayed neutron data and the other on photonuclear data and photon strength functions.

2. Beta-delayed neutron emission data
Beta-delayed neutron emission plays an important role in a wide range of applications such as kinetics and safety operation of reactors, planning of future advanced fuel technology, and calculating anti-neutrino spectra from reactors. It also affects the abundances of the heavy elements produced by the r-process nucleosynthesis, and is the main decay process of very
neutron-rich and unstable nuclei near the driplines. Although half-lives and beta-delayed neutron emission probabilities $P_n$ of individual precursors are available in several compiled and evaluated libraries such as ENSDF, NUBASE, NuDat, etc., there is no complete documentation of measurements and evaluation procedures for these properties. Previous dedicated compilations and evaluations are incomplete and outdated. As for measured neutron spectra, they are not available in any of the mentioned databases.

Integral delayed neutron properties have been studied since the early 1950s’ as they are crucial for determining the reactor kinetics and reactivity. Several measurements of delayed neutron emission curves produced from thermal neutron-induced fission of $^{235}\text{U}$ were performed and were fitted by grouping the delayed-neutron emitters in six groups according to their half-lives. An international group formed under the auspices of NEA-OECD (Subgroup-6) [4], however, concluded that the measured reactivity curves were improved by expanding the 6-group model to an 8-group by separating the three longest-lived delayed neutron precursors ($^{85}\text{Br}$, $^{137}\text{I}$, and $^{88}\text{Br}$) into single groups. However, the uncertainties in the delayed-neutron data remained an issue.

To address the above-mentioned gaps and data needs, the IAEA coordinated an international project (CRP) with the aim of creating a Reference Database of beta-delayed neutron data [5]. The scope of the CRP (2013-2018) [6] covered the following items:

- Compilation and evaluation of experimental half-lives and $P_{\alpha\beta}$ for delayed-neutron precursors,
- Establishing standards in different mass regions, for which several independent and reliable measurements are available,
- Developing new empirical systematics based on the new evaluated $P_n$ data,
- Calculating beta-decay half-lives and $P_n$ values using available empirical and microscopic models,
- Testing the new evaluated beta-decay half-lives and $P_n$ values against macroscopic data and benchmark experiments,
- Measuring total delayed neutron yields (TDN) and spectra for a range of actinides,
- Re-evaluating 6- and 8-group representations based on new measurements, and
- Developing systematics for 6- and 8-group representations.

Fourteen groups from different institutes and countries participated in the CRP. The details of the work and the results are discussed in a comprehensive article submitted to Nuclear Data Sheets [7]. The new Reference Database is available on the IAEA server at www-nds.iaea.org/beta-delayed-neutron/database.html and consists of a microscopic and a macroscopic section.

2.1. Compilation and evaluation

For the purposes of the CRP, all experimental data on individual precursors that were published until May 2018 were considered. Beta-decay half-lives and beta-delayed neutron emission probabilities $P_n$ were compiled and evaluated for 649 beta-delayed neutron emitters, of which 221 were in the lighter mass region ($Z < 29$) while 428 were in the fission mass region ($Z > 28$). For each one of these nuclides, the available experimental data and methods were assessed before the most reliable data were selected for the averaging procedure which resulted in the recommended value. The evaluated data were published in two separate articles, one for the lighter mass region ($Z < 29$) [8] and one for the higher fission mass region ($Z > 28$) [9], respectively.

The new evaluated data ($T_{1/2}, P_n$) were then used to determine systematic trends using three different empirical formulas: Kratz and Herrmann [10], McCutchan et al. [11] and Miernik [12]. As these systematics showed considerable scatter, the corresponding systematics along a given
Z were found to be more compact and were consequently used to identify outliers that needed to be investigated [9].

2.2. Summation calculations
The new evaluated \( (T_{1/2}, P_n) \) data for individual precursors were tested against macroscopic data using the summation method. The new emission probabilities \( P_n \) were combined with cumulative fission yields in the summation method to obtain total delayed neutron yields for a wide range of fissioning systems at various energies. The impact of the new CRP data on the total delayed neutron yields is shown in Fig. 1. What is clear from the figure is the calculated total delayed neutron yields are sensitive to the fission yield data and that they agree with the recommended values of Ref. [13] only when JEFF-3.1.1 [14] fission yields are used. From the comparisons it is obvious that fission yield data and libraries need to be investigated thoroughly.

2.3. Benchmarking
Further testing of the new microscopic \( (T_{1/2}, P_n) \) data was performed by comparing them with well-defined benchmark experiments that have measured certain important properties of the reactor with high precision. These reactor parameters are: \( \beta \), the fraction of delayed neutrons in the reactor core at creation (at high energies), \( k_{eff} \), the reactor averaged multiplication factor (a measure of criticality), and \( \beta_{eff} \) which is the effective delayed neutron fraction (fraction of new fissions initiated by delayed neutrons).

The neutron transport code MCNP (6.1.1b version) was used to compute \( k_{eff} \) and \( \beta_{eff} \) for eight different integral experiments:

- fast systems with integral data for \( k_{eff} \) and \( \beta_{eff} \) (very few integral data for \( \beta_{eff} \) available)
- systems that are sensitive to \(^{233}\text{U}, {^{235}\text{U}, {^{238}\text{U} and} {^{239}\text{Pu}} isotopes.

All the information about the integral experiments was taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [18] and the International Reactor Physics Experiment Evaluation (IRPhE) handbooks [19].

The nuclear data libraries that were used in the summation calculations were JEFF-3.1.1 [14] and ENDF/B-VII.1 [20]. Three calculations were performed each time, one using the standard library data for total neutron yields and delayed neutron yields, a second time (v01) replacing the total neutron yields and total delayed neutron yields by the values obtained from the summation method using the library decay data, and a third time (v02) replacing the total neutron yields and delayed neutron yields by the summation method values using the CRP evaluated data \( (T_{1/2}, P_n) \). The results for all eight integral experiments for \( k_{eff} \) are shown in Fig. 2. From the figure, it is clear that ENDF/B-VII.1 standard and v01 results agree with experimental values within 1 standard deviation, ENDF/B-VII.1 v02 deviates from experimental values for \(^{235}\text{U} \) integral experiments, the JEFF-3.1.1 standard results are scattered, while the results for JEFF-3.1.1 v01 and v02 closely agree with the standard. The corresponding results for \( \beta_{eff} \) are shown in Fig. 3. In this case, the results obtained with the CRP data deviate significantly for both ENDF/B-VII.1 and JEFF-3.1.1 libraries.

3. Photonuclear data and Photon Strength Functions
Photon strength functions and photonuclear cross sections are necessary for applications such as radiation shielding and transport analyses, radiation dosimetry, fission and fusion technologies, safeguards and inspection technologies, transmutation of nuclear waste and nuclear astrophysics. In recent years, a lot of effort has been made to measure gamma-ray data related to photonuclear reactions and photon strength functions that needs to be compiled, evaluated, and disseminated to the user community.
Figure 1. Total delayed neutron yields calculated using the summation method for thermal n-induced fission of $^{235}$U. The different symbols are obtained using different $P_n$ compilations: Wilson and England [15] (red circles), Rudstam et al. [16] (blue triangles), Pfeiffer et al. [17] (magenta triangles), CRP data [7] (green diamonds). The fission yield data were obtained from the evaluated libraries ENDF/B-VII.1, JENDL-4.0, and JEFF-3.1.1. Figures provided courtesy of V. Piksaikin (IPPE.)

An international effort under an IAEA Coordinated Research Project (CRP) [21] (2016-2019) with the objective of updating the photonuclear data library and generating a Reference Database for Photon Strength Functions has recently concluded [22]. Sixteen groups from different institutes from all over the world participated in this project. The two distinct parts of the CRP are summarized in the following sections.

3.1. Photonuclear data library
The IAEA Photonuclear data library (http://www-nds.iaea.org/photonuclear) [23] includes photoabsorption cross sections, total and partial photo-neutron reaction cross sections, and neutron emission energy spectra for 164 isotopes. Since its release in 1999, new data have been measured, improved evaluation techniques and theories have been developed and new
Figure 2. Ratio of calculated over measured $k_{\text{eff}}$ values for several actinides. Plotted are the results obtained with ENDF/B-VII.1 standard (blue circles), ENDF/B-VII.1 v01 (black circles), ENDF/B-VII.1 v02 (green circles) and with JEFF-3.1.1 standard (red diamonds), JEFF-3.1.1 v01 (magenta diamonds) and JEFF-3.1.1 v02 (cyan diamonds). Figure provided courtesy of D. Cano-Ott (CIEMAT).

Figure 3. Same as Fig. 2 but for $\beta_{\text{eff}}$. Figure provided courtesy of D. Cano-Ott (CIEMAT).

measurement techniques aiming at resolving the existing discrepancies have emerged.

The IAEA CRP has updated the library by revising the existing evaluations and adding new evaluations of isotopes that were not included before. Additionally, photo-production of isotopes of interest to medical applications have also been considered, such as isotopes produced by $\gamma + ^{39,41}$K, $^{186}$Re produced via $^{187}$Re($\gamma,n)^{186}$Re for which data exist. In total, 219 nuclides
are included in the new library, among which 55 are new. Out of the 219 evaluations, 188 were performed by the CRP evaluators, 20 were kept from the previous 1999 library and one was taken from JENDL/PD-2016.

The new evaluation approaches, models and codes used in the project as well as selected results are presented in a comprehensive article [24]. The new library has been assembled and verified and is available at the IAEA web server (URL: http://www-nds.iaea.org/endf/). In addition, GDR parameters have been extracted by fitting Lorentzian-type curves to a revised database of experimental photoabsorption and photoneutron cross-section data published up to June 2018. The new compilation is an extension and improvement of earlier compilations and also includes recommendations [25, 26].

3.2. Photon Strength Functions database
Photon strength functions (PSF) extracted from different measurements have been compiled and assessed. The compilation includes data in the GDR region and in the range near and below the neutron separation energy, including average resonance capture data, NRF, proton-capture and inelastic scattering data and other charged-particle reaction data (Oslo method). The data have been assessed to ensure compatibility near the neutron thresholds, as well as to resolve discrepancies observed between different types of measurements and extraction methods, such as the NRF and Oslo methods. Global models (Lorentzian-type SMLO [27], QRPA [28]) have also been developed in the entire energy range and have been compared with all the compiled PSF data. In addition, the global models have been tested against 1) singles γ-ray spectra from thermal neutron capture yielding information on the PSF , 2) multi-step cascade spectra from individual neutron resonances, 3) two-step cascade spectra following thermal neutron capture, 4) average radiative width <Γγ> and 5) Maxwellian-averaged cross sections at 30 keV yielding information on the integrated PSF below the neutron separation energy.

A detailed report on the compilation, assessment, modeling and validation of the PSF data, as well as on the contents of the new PSF database has been published in Ref. [29]. The data will be available for downloading at the IAEA web server (URL: http://www-nds.iaea.org/PSFdatabase).

4. Conclusions
The compilation, evaluation and dissemination of nuclear data relies heavily on international collaboration. We have presented two international projects coordinated by the IAEA with the purpose of developing and disseminating nuclear data that are important for both basic sciences and applications. The products of these projects, namely, the Reference Database for beta-delayed neutrons, the new IAEA Photonuclear Data Library 2019, as well as the Reference Database for Photon Strength Functions, are expected to be widely used by the user community at large.

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