NUCLEAR ENERGY AND ASTROPHYSICS APPLICATIONS OF ENDF/B-VII.1 EVALUATED NUCLEAR LIBRARY

Boris Pritychenko

National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY, USA

Recently released ENDF/B-VII.1 evaluated nuclear library contains the most up-to-date evaluated neutron cross section and covariance data. These data provide new opportunities for nuclear science and astrophysics application development. The improvements in neutron cross section evaluations and more extensive utilization of covariance files, by the Cross Section Evaluation Working Group (CSEWG) collaboration, allowed users to produce neutron thermal cross sections, Westcott factors, resonance integrals, Maxwellian-averaged cross sections and astrophysical reaction rates, and provide additional insights on the currently available neutron-induced reaction data. Nuclear reaction calculations using the ENDF/B-VII.1 library and current computer technologies will be discussed and new results will be presented.

1. Introduction

The value of compilation, evaluation and computer storage of neutron cross sections was first recognized in the early 50's [1] prompted by the urgent needs of nuclear industry. These cross sections were first summarized in the BNL-325 report and Evaluated Nuclear Data File (ENDF) library [2 - 4]. In present days, evaluation and dissemination of nuclear reaction data are coordinated by the CSEWG and the U.S. Nuclear Data Program in USA and by the Working Party on International Nuclear Data Evaluation Cooperation worldwide. Over the years, the nuclear data activities were extended to all low- and intermediate-energy nuclear physics.

The rapid access to the latest data is based on the database storage and worldwide dissemination that relies on the presently available technologies [5] and data formats. Nowadays, size and representation of nuclear data files are no longer limited by the computer hardware and software and a collaborative effort is underway to convert nuclear data from the historic 80-character-long records to XML format.

For years, nuclear data field improvements were driven by nuclear science and technology applications. These activities evolved over the years and lead to the release of the ENDF/B-VII.1 evaluated library in December of 2011 [4]. The overall nuclear data maturation and modern computer technologies created many new opportunities for nuclear reaction calculations, data mining and analysis. In this work, I will concentrate on selected nuclear reactor operation and astrophysics integral quantities that can be extracted from the ENDF/B-VII.1 library.

2. Evaluated Nuclear Reaction Data Libraries

Increasing energy demand, concerns over climate change and dependence on overseas supplies of fossil fuels are coinciding to make the strong case for increasing use of nuclear power. Presently, ~20 % of U.S. electrical power is generated by 104 nuclear power plants. These plants provide ~75 % of non-emission generated electricity in the country. Ongoing construction and design of the new power units, 55 worldwide and 6 in the USA, require constant improvements of evaluated nuclear reaction data that are absolutely essential for reactor operations.

All evaluated nuclear reaction data files are assembled using the internationally adopted ENDF-6 format [6]. This format, maintained by CSEWG, provides the foundation for ENDF libraries. ENDF is a core nuclear reaction library containing evaluated (recommended) cross sections, neutron spectra, angular distributions, fission product yields, thermal neutron scattering, photo-atomic and other data, with emphasis on neutron-induced reactions.

In the present work, the author considers neutron elastic scattering (n,n), capture (n, γ) and fission (n, f) reactions and several integral values that are of importance for nuclear science and technology applications. Integral values of thermal neutron cross sections (σ^{2200}), Westcott factors (g^{w}), resonance integrals (RI), Maxwellian-averaged cross sections (σ^{Maxw}) and astrophysical reaction rates (*R(T9)*) were calculated in a systematic approach for Z = 1 - 100 nuclei (materials) using the nuclear reaction data, Doppler broadened at multiple temperatures. Finally, I will use these values for benchmarking and validation of the ENDF/B-VII.1 library.

2. Thermal Neutron Cross Sections, Westcott Factors, Resonance Integrals, Maxwellian-Averaged Cross Sections and Astrophysical Reaction Rates

Calculations of Westcott factors, resonance integrals, Maxwellian-averaged cross sections and reaction rates using the evaluated neutron library data have been performed. Since neutron thermal cross sections in the lab reference system are tabulated in Doppler-broadened ENDF evaluations, the author simply extracted these values from the ENDF/B-VII.1 library.

Westcott g-factor is the ratio of Maxwellian-averaged cross section to the 2200 m/s (thermal) cross section

$$g^{w} = \sigma^{Maxw}/\sigma^{2200}. \quad (1)$$

The epicadmium dilute resonance integral (RI) for a particular reaction σ(E) in 1/E spectrum is expressed by

$$RI = \int \sigma(E)/E\, dE, \quad (2)$$

where the lower integration limit E_c is determined by cadmium cutoff energy ($E_c = 0.5$ eV) and the upper limit is often chosen as ∞ [2].

Average cross sections for Maxwellian spectrum temperature (*kT*) [7] are defined as

$$\sigma^{Maxw}(kT) = <\sigma v>/v_T, \quad (3)$$

where v is the relative velocity of neutrons and a target nuclide and v_T is the mean thermal velocity given by $v_T = \sqrt{2\,kT/\mu}$, where μ is the reduced mass.

The astrophysical reaction rate, R, is defined as

$$R = N_A <\sigma v>, \quad (4)$$

where N_A is the Avogadro number. To express reaction rates in [cm3/mole s] units, an additional factor of 10^{-24} can be introduced. Temperature (*kT*) , in units of energy (*e.g.* MeV) is related to that in Kelvin (*e.g.* 10^9 K) as $T_9 = 11.6045\ kT$. These equations were used to calculate integral values using the original evaluated neutron data from the ENDF/B-VII.1 library within the typical range of energies.

3. Results and Discussion

Due to space limitations, only selected data sets are discussed in the current proceedings. The complete sets of ENDF/B-VII.1 thermal neutron cross sections, Westcott factors, resonance integrals, Maxwellian-averaged cross sections and astrophysical reaction rates are available in the Brookhaven report [8].

3.1. Neutron Thermal Cross Sections

ENDF/B-VII.1 thermal cross section ratio for neutron fission are shown in Fig. 1. Using the method of visual inspection one can notice deviations for light and medium nuclei and minor actinides evaluations. In the minor actinide region, deviations are actually in the JENDL-4.0 evaluations, since these were adopted by ENDF/B-VII.1 library.

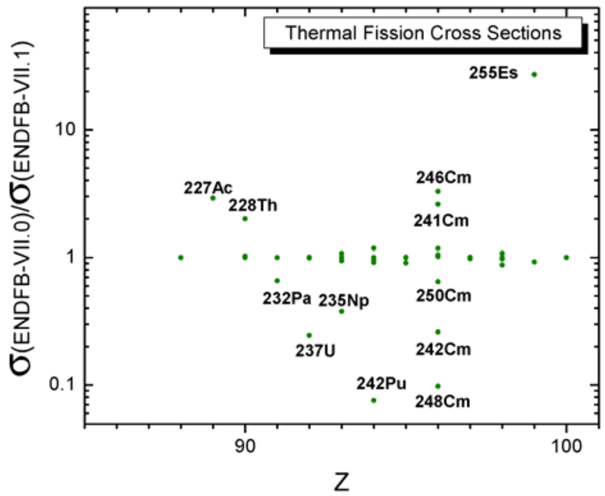

Fig. 1. Ratio of thermal neutron fission cross sections for ENDF/B-VII.0 to ENDF/B-VII.1 [3, 4]. Where discrepancies are evident, ENDF/B-VII.1 values are thought to be more accurate.

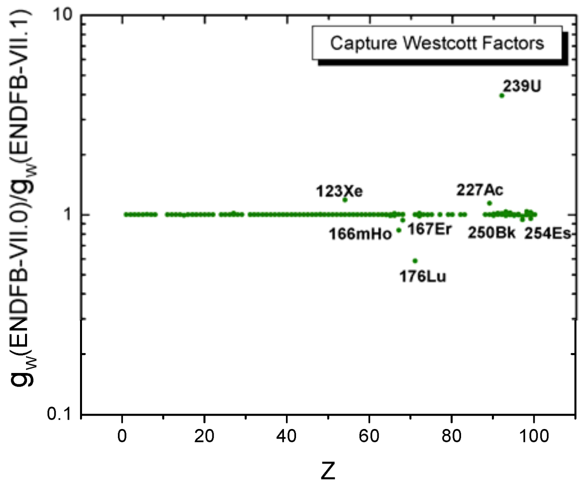

Fig. 2. Ratio of thermal neutron capture Westcott factors for ENDF/B-VII.0 to ENDF/B-VII.1 libraries [3, 4].

3.2. Westcott Factors

Complete calculation of capture and fission Westcott factors reveals that most of them are close to 1 with an exception of non-1/v σ(n, γ) nuclei: ^{113}Cd, ^{135}Xe, ^{149}Sm, ^{151}Eu, ^{176}Lu, ^{182}Ta, ^{239}Pu, ^{243}Am [2]. The ENDF/B VII.0/VII.1 capture Westcott factors ratio is shown in Fig. 2.

3.3. Resonance Integrals

The ratio of Atlas of Neutron Resonances recommended neutron capture resonance integrals [2] to ENDF/B-VII.1 calculated values within the 0.5 eV - 20 MeV range of energies is shown in Fig. 3. Several data outliers in this case could be traced to the lack of measurements and incomplete overlap of experimental and theoretical data for ^{17}O, ^{166m}Ho and ^{46}Ca, ^{204}Hg, respectively. However, there are neutron capture cross section deficiencies in the minor actinide evaluations of the ^{233}Th, ^{251,253}Cf and ^{254,254m}Es.

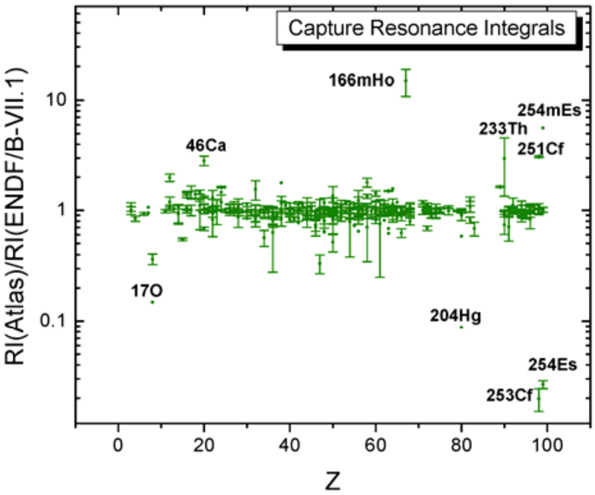

Fig. 3. Ratio of neutron capture resonance integrals for Atlas of Neutron Resonances [2] to ENDF/B-VII.1 [4].

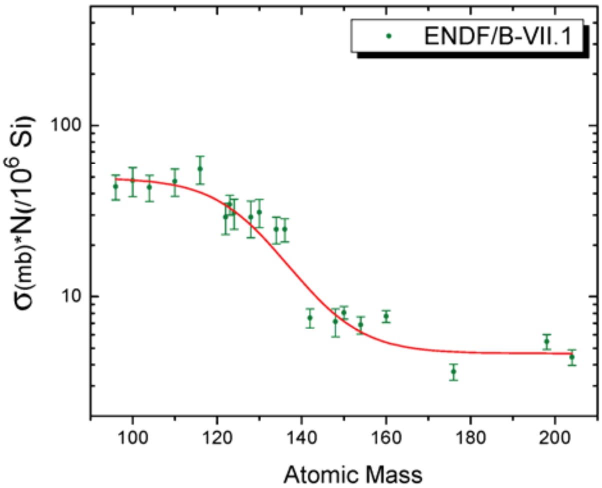

Fig. 4. ENDF/B-VII.1 library product of neutron-capture cross section (at 30 keV in mb) times solar system abundances (relative to Si = 10^6) as a function of atomic mass for nuclei produced only in the *s*-process.

3.3. Maxwellian-averaged Cross Sections and Astrophysical Reaction Rates

The slow-neutron capture (*s*-process) is responsible for creation of ~50 % of the elements beyond iron. In this region, neutron capture becomes dominant because of the increasing Coulomb barrier and decreasing binding energies. This *s*-process takes place in the Red Giants and Asymptotic Giant Branch stars, where neutron temperature (*kT*) varies from 8 to 90 keV.

It is commonly known that for the equilibrium *s*-process-only nuclei product of $\sigma^{Maxw}(kT)$ and solar-system abundances (n_A) is preserved

$$\sigma_A \, n_A = \sigma_{A-1} \, n_{A-1} = constant. \quad (5)$$

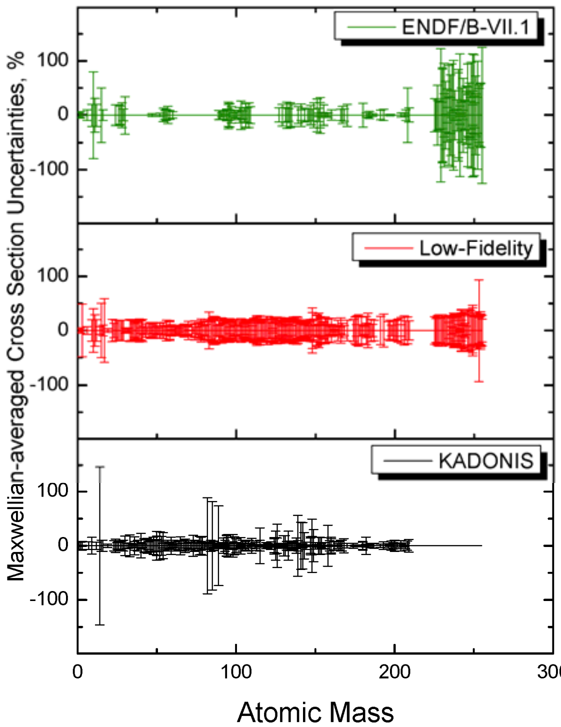

Fig. 5 Maxwellian-averaged Neutron Capture Cross Section Uncertainties for ENDF/B-VII.1 library, Low-Fidelity project and KADONIS database [4, 9, 10].

To verify this phenomenon, the calculated σ^{Maxw}(30keV) from the ENDF/B-VII.1 library were multiplied by solar abundances and plotted in Fig. 4. Visual inspection of the Fig. 4 indicates two local equilibrium and ledge-precipice break at A ~ 138 for the ENDF/B-VII.1 fit and relatively high value for ^{116}Sn. This phenomenon is due to the fact that ^{116}Sn solar abundance has *r*-process contribution. Astrophysical reaction rates and their uncertainties for the whole range of ENDF nuclei have been calculated and listed in the BNL report [8].

Additional *s*-process nucleosynthesis data could be interactively calculated and downloaded from the NucRates Web application *http://www.nndc.bnl.gov/astro*. These complimentary data sets demonstrate a strong correlation between nuclear astrophysics and nuclear industry data needs the large nuclear astrophysics potential of ENDF libraries, and a perspective beneficial relationship between both fields.

3.4. Cross Section Uncertainties

To gain better understanding of ENDF/B-VII.1 library integral values and their uncertainties, the Low-Fidelity covariances [9] were investigated. These results together with KADONIS data [10] are shown in Fig. 5.

4. Conclusion & Outlook

Increasing demands for development of new nuclear energy and astrophysics applications provided a strong motivation for this work. A complete calculation of Westcott factors, resonance integrals, Maxwellian-averaged cross sections, astrophysical reaction rates and their uncertainties has been performed. Neutron thermal cross section data were extracted from the ENDF libraries. Present data were analyzed using benchmarks, where available.

Data analysis indicates substantial progress in the improvements in the ENDF/B-VII.1 library's quality and its importance for a wide variety of applications.

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