Outline of Evaluations for JENDL-3.3

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Evaluation for JENDL-3.3 was performed by considering the accumulated feedback information and various benchmark tests of the previous library JENDL-3.2. The major problems of JENDL-3.2 were solved with the new library. This paper describes what was done for JENDL-3.3.

1. Introduction

The JENDL-3.2 data [1] have been used in various application fields since the library was released in 1994. However, some drawbacks of the library were pointed out by comparing with differential and integral measurements. The evaluation work for JENDL-3.3 started in 1997 in order to remove the drawbacks. The compilation of the new library was finished in March 2002, and then it was officially released in May 2002 as JENDL-3.3, which provides the neutron-induced reaction data for 337 nuclides in the incident energy region from 10^{-5} eV to 20 MeV.

This paper briefly describes the data for light & medium-heavy nuclides, heavy nuclides, and minor actinides, together with covariances.

2. Summary of the Problems in JENDL-3.2

The major problems of JENDL-3.2 are summarized as follows:

(1) There exists a large difference in the criticalities of light water reactors between the JENDL-3.1 [2] and -3.2 calculations. The JENDL-3.2 values are by 0.3-1.1% larger than those of JENDL-3.1 for thermal reactors.

(2) It was found that the JENDL-3.2 calculations yield by 0.7-1.3% larger criticalities for fast cores which contain ^{233}U.

(3) Energy distributions of secondary neutrons were found to be incorrect for several heavy nuclei.

(4) There is inconsistency between elemental and isotopic data for medium-heavy nuclides.

(5) In the MeV region, capture cross sections of many nuclei decrease rapidly with incident

energy, which is not likely to occur.

(6) Covariances are needed for several important nuclei.

3. Evaluation

3.1 Light and Medium-heavy Nuclide Data

(1) Resolved Resonance Parameters

Resolved resonance parameters were revised for V, ^{46,48,49,50}Ti, ^{50,52,53,54}Cr, ^{54,56}Fe, ^{58}Ni, ^{59}Co, ^{99}Ru, and ^{186}W by examining experimental data. The resolved resonance parameters of ^{56}Fe were taken from JEF-2.2 [3] with the Reich-Moore formalism. As for ^{186}W, it was pointed out that the capture resonance integral of JENDL-3.2 (347.0 b) is too small as compared with the value of 485.0±15.0 b recommended by Mughabghab [4]. In the JENDL-3.3 evaluation, the parameters at the 18.8-eV resonance were modified and a negative resonance was deleted. As a result, the resonance integral led to a larger value of 528 b, being consistent with a value of 510.7±24.3 b measured by Kobayashi *et al*. [5]

(2) Total Cross Sections

Elemental data files were not produced in order to avoid the inconsistency between the elemental and isotopic data seen in JENDL-3.2. However, there are a lot of measured total cross-section data on natural elements in the MeV region. These measurements were taken into account in the present evaluation. In principle, a weighted sum of the evaluated cross section of an isotope should reflect the measured total cross section of the element. For instance, in the MeV region, the total cross sections of ^{57,58}Fe were obtained from the optical model calculations, while that of ^{54}Fe was derived from the measurements [6,7]. The total cross section of elemental iron was evaluated on the basis of the experimental data [8-10] in the energy region from 700 keV to 20 MeV. Then, the total cross section of ^{56}Fe was obtained by subtracting the contributions of ^{54,57,58}Fe from the cross section of elemental iron.

(3) Reaction Cross Sections

The cross sections of ^{162,164,166,167,168,170}Er were evaluated mainly by nuclear model calculations. The optical model parameters were obtained so as to reproduce the measured total cross sections of elemental erbium. The capture cross sections of ^{166,167,168,170}Er measured by the Tokyo Institute of Technology group [11-13] were taken into account in the present evaluation.

(4) Gamma-ray Production and Double-differential Neutron Emission Cross Sections

In JENDL-3.2, gamma-ray production data were included for 66 nuclides. However, no isotopic data were available for 9 elements: Mg, S, K, Ti, Cr, Mo, Cd, Eu, and W. The gamma-ray production cross sections and emitted gamma-ray spectra for the isotopes of these elements were calculated by using the SINCROS code system [14] for JENDL-3.3.

Double-differential neutron emission cross sections, *i.e.*, angle-dependent neutron emission spectra, were not contained in JENDL-3.2. In the present work, the double differential cross sections were included for 60 nuclides; most of them were taken from JENDL/F-99 [15].

(5) Cross Sections of Light Nuclei

Minor modification was made for the cross sections of ^{11}B, C, ^{14,15}N, and ^{16}O. According to the preliminary benchmark analyses of the thermal critical assemblies (STACY and TRACY) with uranyl nitrate solution, the (n,p) cross section of ^{14}N was found to be too small at the thermal energy. The JENDL-3.3 evaluation adopted Mughabghab's recommendation [16], which led to an improvement of criticality values for the STACY and TRACY cores. As for the ^{15}N(n,γ) reaction that is important for *s*-process nucleosynthesis, the *p*-wave capture contributes to cross sections predominantly above 10 eV, although the JENDL-3.2 cross sections exhibit an inverse of velocity behavior up to 10 keV. We adopted the cross-section formula obtained by Meissner *et al*. [17] for JENDL-3.3.

3.2 Heavy Nuclide Data

(1) Resonance Parameters and Prompt Fission Neutron Spectra for ^{235}U

The overestimation of k_{eff} is the biggest problem concerning JENDL-3.2 when the library is applied to thermal fission reactors. In order to solve this problem, we re-evaluated the resonance parameters of ^{235}U and the prompt fission neutron spectra from ^{235}U. The resonance parameters were replaced with those obtained by Leal *et al*. [18] The fission neutron spectra were re-evaluated by Ohsawa [19] with a multi-modal fission analysis.

(2) Simultaneous Evaluation of Fission Cross Sections

Fission cross sections above the resonance region are also important for reactor calculations. We adopted a simultaneous evaluation [20] to obtain the fission cross sections of major actinides above 30 keV. The experimental data on ^{233}U were included in the present evaluation, while the ^{233}U data were evaluated separately from the simultaneous evaluation for JENDL-3.2. The fission cross sections of ^{233}U obtained for JENDL-3.3 are lower than those for JENDL-3.2 in the energy range above several hundred keV.

(3) Secondary Neutron Spectra

Secondary neutron spectra for the (n,n'), (n,2n), and (n,3n) reactions compiled in JENDL-3.2 have been criticized for a long time. We performed spectrum calculation with the GNASH code [21] and the results were processed with GAMFIL code [22]. With this procedure, the crucial problems concerning the energy distributions of secondary neutrons were obviously solved.

(4) Direct/Semi-direct Capture

In the JENDL-3.2 evaluation, the capture cross sections at higher energies were often ignored, because these cross sections became extremely small when the Hauser-Feshbach statistical model was used to calculate them. It is known that the direct/semi-direct (DSD) capture model should be applied to calculate capture cross sections in this energy region. In the present work, we took account of the DSD contributions.

(5) Delayed Neutrons

The number of delayed neutrons per fission for ^{235}U and ^{238}U were re-evaluated on the basis of available experimental data.. It was found that the re-evaluated results are consistent with the values obtained by Sakurai and Okajima [23] considering the integral measurements at FCA, TCA, and MASURCA. The delayed neutron spectra were taken from the summation calculation results obtained by Brady and England [24] for six temporal groups.

3.3 Minor Actinide Data

(1) ^{237}Np

The resonance parameters were revised on the basis of the new experimental data obtained at CEA Saclay [25]. As a result, the upper boundary of the resolved resonance region was extended from 130 eV to 500 eV. In the energy range above the resonance region, the total, inelastic scattering, capture and (n,3n) reaction cross sections were replaced with the new evaluation by Ignatyuk *et al*. [26] The fission cross section was obtained by least-squares fitting to experimental data. The (n,2n) reaction cross section is the same as that given in JENDL-3.2.

(2) ^{241}Am

The resonance parameters of Maslov *et al*. [27] were modified so as to reproduce slightly larger thermal cross sections. The present evaluation gives a capture cross section of 639.47 b at 0.0253 eV which is 6.6% larger than JENDL-3.2. The fission cross section above 100 keV was obtained by fitting to experimental data. The evaluation of Maslov *et al*. was adopted for the capture, (n,2n), (n,3n) and inelastic scattering cross sections. For the capture cross section, the isomeric ratio was evaluated from experimental data and the GNASH calculations, as seen in Fig. 1.

3.4 Covariance Data

The previous library JENDL-3.2 contains covariance data only for ^{55}Mn, although we were requested to prepare covariances for the nuclides which were required to evaluate the characteristics of fast reactors. In order to meet the needs, covariance data were evaluated for selected nuclides in JENDL-3.2, and they were made available as the JENDL-3.2 Covariance File [28]. These covariance data were obtained from measurements or nuclear model calculations which the evaluated mean data were based on. Most of the covariance data were also adopted in JENDL-3.3 with a slight modification.

The simultaneous evaluation yielded the covariance matrices for the fission cross sections of $^{233,235,238}U$ and $^{239,240,241}Pu$ in the energy region above several tens of keV. The matrices represent not only the correlation of individual fission cross sections between different incident energies but also that of a fission cross section with another fission cross section.

In JENDL-3.3, covariances are included for 20 nuclides. The covariances for ^{48}Ti, V, and ^{59}Co were newly evaluated for JENDL-3.3.

4. Conclusions

Evaluation and compilation were performed for JENDL-3.3. Only the significant changes from JENDL-3.2 were described in this report, although data for more than a hundred nuclides were revised. The major problems of JENDL-3.2 were solved with the present library.

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References

[1] T. Nakagawa, *et al*.: J. Nucl. Sci. Technol., **32**, 1259 (1995).
[2] K. Shibata, *et al*.: JAERI 1319 (1990).
[3] C. Nordborg, M. Salvatores: Proc. Int. Conf. on Nuclear Data for Science and Technology, Gatlinburg 1994, Vol. 2, p.680 (1994).
[4] S.F. Mughabghab: "Neutron Cross Sections," Vol. 1, Part B, Academic Press (1984).
[5] K. Kobayashi, *et al*.: Proc. Conf. Neutron Physics, Kiev 1987, Vol. 4, p. 238 (1988).
[6] E.M. Cornelis, *et al*.: Proc. Int. Conf. Nuclear Data for Science and Technology, Antwerp 1982, p.135 (1983).
[7] R.F. Carlton, *et al*.: Bull. Am. Phys. Soc., **30**, 1252 (1985).
[8] K. Berthold, *et al*.: Proc. Int. Conf. Nuclear Data for Science and Technology, Gatlinburg 1994, Vol. 1, p.218 (1994).
[9] A.D. Carlson, R.J. Cerbone: Nucl. Sci. Eng., **42**, 28 (1970).
[10] F.G. Perey, *et al*.: ORNL-4823 (1972).
[11] A.K.M. Harun-ar-Rashid: Ph.D. Thesis, Tokyo Institute of Technology (2000).
[12] A.K.M. Harun-ar-Rashid, *et al*.: J. Nucl. Sci. Technol., **37**, 421 (2000).
[13] M. Igashira: Private communication (2002).
[14] N. Yamamuro: JAERI-M 90-006 (1990).
[15] S. Chiba, *et al*.: J. Nucl. Sci. Technol., **39**, 187 (2002).
[16] S.F. Mughabghab, *et al*.: "Neutron Cross Sections," Vol. 1, Part A, Academic Press (1981).
[17] J. Meissner, *et al*.: Phys. Rev., **C53**, 977 (1996).

[18] L.C. Leal, *et al*.: Nucl. Sci. Eng., **131**, 230 (1999).
[19] T. Ohsawa: JAERI-Conf 2001-006, p.157 (2001).
[20] T. Kawano, *et al*.: J. Nucl. Sci. Technol., **37**, 327 (2000).
[21] P.G. Young, E.D. Arthur: LA-6947 (1977).
[22] K. Hida: JAERI-M 86-150 (1986) [in Japanese].
[23] T. Sakurai, S. Okajima: J. Nucl. Sci. Technol., **39**, 19 (2002).
[24] M.C. Brady, T.R. England: Nucl. Sci. Eng., **103**, 129 (1989).
[25] V. Gressier, *et al*.: Annals Nucl. Energy, **27**, 1115 (2000).
[26] A.V. Ignatyuk, *et al*.: ISTC-304-95 (1997), and private communication (1999).
[27] V.M Maslov, *et al*.: INDC(BLR)-005 (1996).
[28] K. Shibata, *et al*.: J. Nucl. Sci. Technol., **Suppl. 2**, 40 (2002).

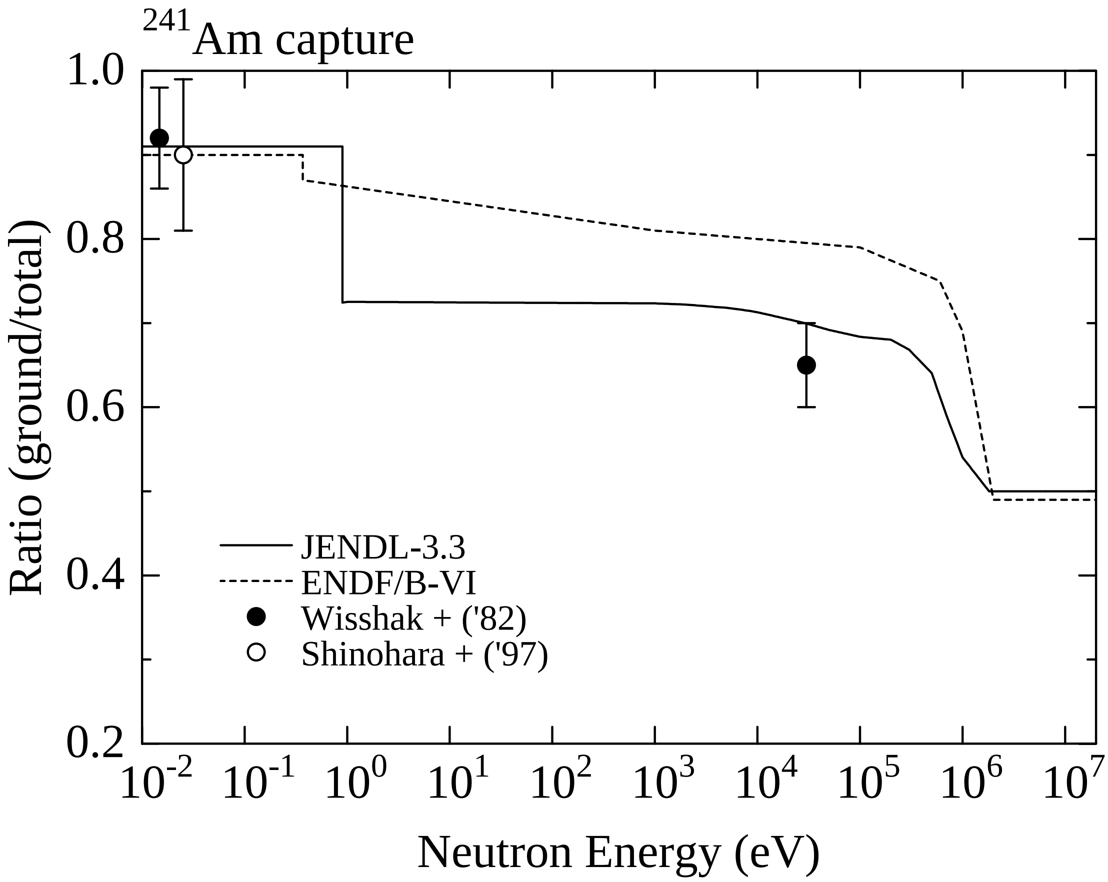

Fig. 1 Ratio of Ground-state Transitions to Total Capture Cross Section of ^{241}Am