

History of FP Nuclear Data Evaluation

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Abstract

The fission product (FP) nuclear data of the JENDL library has been evaluated by FP Nuclear Data Working Group of JNDC for 172 nuclides from As-75 ($Z=35$) to Tb-159 ($Z=65$) for about 30 years since 1971. The working group was organized by total 29 members and initially lead by late Dr. Shungo Iijima. The fission product data were updated in the following sequence: JENDL-1 (28 nuclides) in 1975, JENDL-1.5 (34 nuclides) in 1977 (not released), JENDL-2 (100 nuclides) in 1985, JENDL-3.1 (172 nuclides) in 1990, JENDL-3.2 (172 nuclides) in 1995. The latest version JENDL-3.3 was released in 2002 contains total 337 nuclides. The 172 FP nuclides among them were evaluated by the Working Group with an assistance of the Nuclear Data Center of JAERI. The working group made a validation of the evaluated cross sections through integral tests for the STEK reactivity worth experiments, the CFRMF and EBR-II experiments for capture reactions in standard spectra. We have also participated in the international activities on fission product nuclear data of NEANSC/WPEC: SG-10, 17 and 21.

Introduction

Fission product (FP) nuclear data are important to evaluate a nuclear reactor burn-up performance, reactor dosimetry, nuclear transmutation in fusion reactors and astrophysics research. The evaluation work of FP nuclear data has been made by FP Nuclear Data Working Group^{a)} together with validation of the evaluated data by analyzing the integral experiments performed in reactor core spectra. The latest JENDL library, JENDL-3.3/1/ contains the data for 172 FP nuclides from As-75 to Tb-159. The brief history of the FP nuclear data of JENDL is summarized as follows:

- FPND WG was organized (1971),
- 28 FP nuclides for JENDL-1 FP (completed in 1975) ,
- Additional 34 FP nuclides for JENDL-1.5 FP (1977) (not released),
- 100 FP nuclides for JENDL-2 (1985) ,
- 172 FP nuclides for JENDL-3.1 (1990) ,
- 172 FP nuclides for JENDL-3.2 (1994) .

In each stage, the integral tests were made to validate the evaluated data.

N.B. a) Members of Fission Product Nuclear Data (29 members)

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Fuji Electric: T. Aoki, I. Otake, H. Nakamura
Univ. Tokyo: T. Obata
Hosei Univ.: R. Nakasima
Osaka Univ.: T. Nishigori
NFI: T. Kawamoto
Kyushu Univ.: T. Kawano, Y. Watanabe

History of Evaluation of FP Nuclear Data for JENDL

Evaluation of FP nuclear data for JENDL-1 was started for 27 nuclides important to fast breeder reactor burn up calculations in 1971. They contribute 80% of capture by FP nuclides in a fast breeder reactor. The number of nuclides was increased to 28 soon after. Initially, we had nuclear model codes: statistical model code, RACY/2/, optical model codes: ELIESE-3/3/ and TOTAL. At that time, evaluated data were available only for capture cross sections by Benzi et al./4/ in Italy and AAEC library/5/ in Australia. We aimed at giving all quantities needed for evaluated data file. Accordingly, systematics of nuclear model parameters such as optical model parameters, level density parameters, gamma-ray strength functions were investigated together with level scheme data for the 28 nuclides. The preliminary data for 28 FP were evaluated in the energy range between 100 eV and 15 MeV in 1972/6/. Immediately after a new statistical model code CASTHY was developed by Igarasi/7/, reevaluation was made in the wide energy range from 10^{-5} eV and 20 MeV for the 28 nuclides: Sr-90, Zr-93, Mo-95, Mo-97, Tc-99, Ru-101, Ru-102, Rh-103, Ru-104, Pd-105, Ru-106, Pd-107, Ag-109, I-129, Xe-131, Cs-133, Cs-135, Cs-137, Nd-143, Ce-144, Nd-144, Nd-145, Pm-147, Sm-147, Sm-149, Sm-151, Eu-153, Eu-155. Resonance parameters were taken from the BNL-325 third edition. The results were compiled into JENDL-1 FP data file/8, 9/ in 1975 prior to release of JENDL-1/10/ in 1977. Figure 1 compares the JENDL-1 data with other evaluations and experimental data for Tc-99 and Ag-109.

Since the 28 nuclides were not enough to compose mixed samples used for integral tests, additively the data of 34 nuclides were evaluated. The integral test results/11/ showed large discrepancies between the calculated and measured reaction rates and reactivity worth for several nuclides.

On the other hand, ENDF/B-V was released in 1979. They contained about 200 FP nuclides from Ge-72 to Dy-163/12/. In the Netherlands, RCN-2 files were developed by Gruppelaar/13/. We considered that such a number of FP nuclides as about 200 were not always necessary to analyze reactor burn-up performance. Accordingly, we selected 100 nuclides that gave 99.6% of capture contributions and about 195.4% cumulative fission yields in FBR for JENDL-2/14/. Figure 2 shows the 30 keV neutron capture contributions of the most important 30 nuclides in FBR. The resonance parameters were also evaluated/15/. The JENDL-2 FP data file was completed in 1985 after the general purpose file of JENDL-2 released in 1982/16/. Level density parameters were evaluated from observed resonance level spacings, Dobs, and level scheme data/17/. Optical model parameters/18/ were improved by considering the local systematics of total cross sections, the s- and p-wave neutron strength functions and scattering radii as shown in Fig. 3. This evaluation scheme is called the SPRT method. As for gamma-ray strength functions, we checked consistency between the measured capture cross sections and the integral tests. Figure 4 shows the evaluated capture cross sections of Eu-155. JENDL-2 shows resonance structure, while ENDF/B-V does not.

Integral test of JENDL-2 was made/19/ in 1985 - 1990 for the reactivity worth experiments at the STEK cores/20/ and the capture rate measurements in the standard spectra of CFRMF/21/ and EBR-II/22/. Cross section adjustment tools based on the Bayesian theorem were also developed. Covariance matrixes were calculated taking into account of nuclear model parameter errors, Porter-Thomas distribution for neutron widths, Dyson-Mehta statistics of levels and neutron flux errors. The reliability of the cross section adjustment based on the integral tests was clarified in the case of Zr-93: JENDL-1 cross sections overestimated the reactivity worths by about a factor of 2. Thus, new

evaluation of Zr-93 capture cross sections for JENDL-2 was made by reducing cross section by the factor of 2. Macklin's measurements/23/ reported after the evaluation supported the JENDL-2 as shown in Fig. 5.

Next, evaluation work for JENDL-3 was made aiming at wider applications to thermal reactors, fusion neutronics, reactor dosimetry and astrophysics as well as FBR calculations. In order to save man power, we developed evaluation tools/24/ such as JOBSETTER and its data file of nuclear model parameters to prepare input data for statistical model calculation with CASTHY. Multi-step evaporation and pre-equilibrium code PEGASUS/25/ was effectively used for evaluation of threshold reaction cross sections. Direct inelastic scattering cross sections were calculated with the DWBA code DWUCK-4. Figure 6 shows the evaluation scheme for JENDL-3 by using the various evaluation tools mentioned above. Evaluation of resonance /26/ was accelerated with the REPSTOR and its auxiliary codes developed by Nakawaga/ 27,28/: XTOREP, ETOREP, JCONV and PASSIN etc. New systematics of level density parameters evaluated on the basis of the level scheme data is shown in Fig. 7. Direct inelastic scattering cross sections were considered for even-even nuclides which were belong to nuclides around fission yield peaks and weak absorbing FP nuclides. Figure 8 shows the excitation function of inelastic scattering to the first excited state of Nd-144. The Bayesian adjustment method was adopted to evaluation for capture cross sections of Xe-132, 134 and Eu-152 and 154 for which no experimental data were available. The evaluation of FP nuclear data for JENDL-3.1 was completed in 1990 /29/.

Revision of JENDL-3.1 data was made for JENDL-3.2/30/ by considering new experimental data for 63 nuclides: thermal and resonance parameters for 33 nuclides, capture cross sections for 16 nuclides, direct inelastic scattering cross sections for 8 nuclides, and threshold reaction cross sections calculated with GNASH code for 16 nuclides (which were adopted from JENDL Fusion File) in 1994/31/. Figure 9 shows the typical results of capture cross sections for Cs-137, Sm-144, Sm-148 and Ru-101. For JENDL-3.2, a part of the resonance parameters were improved. As for Ru-101, level scheme data were revised and anomalous behavior of JENDL-3.1 capture cross section around 3 MeV diminished.

Integral tests of JENDL-3.1 and -3.2 showed the C/E values of sample reactivity worths were generally around unity for nuclides lighter than 130 and about 0.9 for heavier nuclides, except for several weakly absorbing nuclides/32,33/ as shown in Fig. 10.

For JENDL-3.3, obvious errors of compilation in JENDL-3.2 were corrected and new evaluations for Tc-99 and Ce-140 were adopted/1/. The data of Zr, Mo, Cd and Sb isotopes and Nb-93 were also revised by adopting the data of the JENDL Fusion File 99.

Activities in WPEC of NEANSC

In 1990's, we participated the activities of Subgroup(SG)10/34/ and SG17/35/ in WPEC of NEANSC. In the SG10 activity investigating evaluation method of inelastic scattering cross sections for FP nuclides and the source of discrepancies of sample reactivity worths for weak absorbing nuclei of the STEK experiments between the measurements and the calculations, in order to answer to Gruppelaar's question/36/, we made the inter-comparison of the evaluated cross sections of JENDL-3.1, ENDF/B-VI and JEF-2/37/. Figure 11 shows an example of the level excitation functions of Mo-96. DEUCK-4 code calculation denoted with a dashed line shows a slightly anomalous behavior for 2.2193 MeV and 2.2345 MeV levels. Further investigation showed that anomalous behavior of the inelastic scattering of nuclides around A=100 came from abnormal p-wave strength functions due to improper optical model

parameters/38/. Figure 12 shows the inelastic scattering cross sections to 535.6 keV level of Mo-100. JENDL-3.2 which shows overestimation was calculated with the DWUCK-4 code using optical model parameters derived from the global fit. On the other hand, Smith's optical model parameters /39/ which were determined by reproducing elastic angular distributions and p-wave neutron strength functions for Zr, Mo, Pd etc. give a good agreement with the experimental data/40/ as shown in the figure. Interpretation of the discrepancies between the differential and integral data for nuclides around the nuclear mass of 100 was made with the rigorous transport calculations /33,41, 42/. Finally, we found probable evidence by the sensitivity study/43/ that the discrepancies came from the adjoint spectrum errors. Figure 13 shows the sensitivity profiles to adjoint spectrum errors (difference between transport calculation spectra /42/ and the ECN ones/20/) in cases of Mo-98 and Ce-140. Sensitivity profile of Mo-98 has a high peak in the high energy region: The effect of the adjoint spectrum error appears as like influence of inelastic scattering uncertainty on reactivity. This result is an answer to Gruppelaar's question. The sensitivity profile of Ce-140 is distributed in the wide energy region. This trend is observed for most weak absorbing FP nuclides except for nuclides around A=100 and standard scattering samples such as oxygen and lead. These nuclides also showed similar discrepancies of reactivity worths as Zr and Mo isotopes. Thus, it has been concluded that poor adjoint spectrum produced the discrepancies of reactivity worth for weak absorbing FP nuclides.

In the SG17, comparison of the integral values such as one-group cross sections and reactivity worth of pseudo FP in a typical FBR core spectrum did not show so large differences between various evaluated data files compared to individual FP nuclides. We found some systematic differences of capture cross sections for important FP nuclides between JENDL-3.2 and JEF-2.2 came from adoption of adjusted cross section: JEF-2.2 adopted adjusted one, but JENDL-3.2 didn't/35/. Accordingly, it was found that there was strong correlation between the C/E values of reactivity worth calculated with JENDL-3.2 and one-group cross section ratios of JENDL-3.2 to JEF-2.2.

Recently, ENDF/B-VI was revised for 19 nuclides by considering new evaluated data of resonance parameters. CENDL-3 for 101 FP nuclides/44/ was compiled in China. SG-21 has been established in 2002 to review the evaluated data stored in JENDL-3.2, ENDF/B-VI.8, JEF-2.2, BROND-2, CENDL-3/45/.

Conclusion

Previous Working Group of FP Nuclear Data continued very long term activity until completion of SG10 activity, although the WG formally finished in 1997 when the integral test of JENDL-3.2 was completed. Recently, partial revision of JENDL-3.2 was made for JENDL-3.3 by the Nuclear Data Center of JAERI. JENDL-3.3 seems to be good, but some parts are worse than CENDL-3 or ENDF/B-VI.8. Therefore, we are going to evaluate FP nuclear data for JENDL-4 by reorganizing the FP Nuclear Data Working Group in JNDC.

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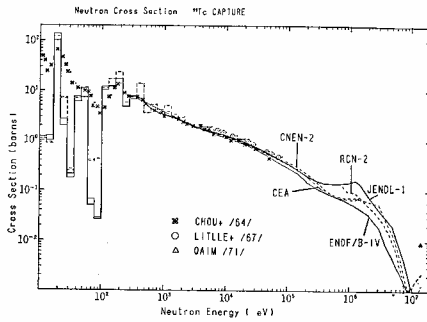


Fig. 3.5.2 Capture cross sections of ⁹⁹Tc.

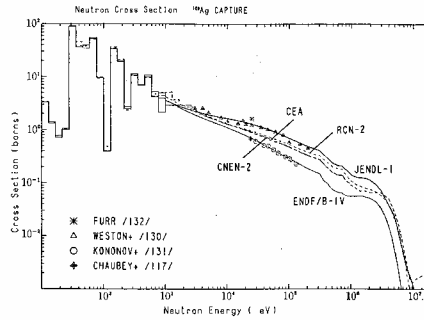


Fig. 3.13.2 Capture cross section of ¹⁰⁹Ag.

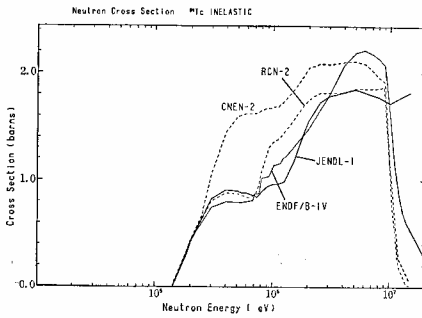


Fig. 3.5.3 Inelastic scattering cross sections of ⁹⁹Tc.

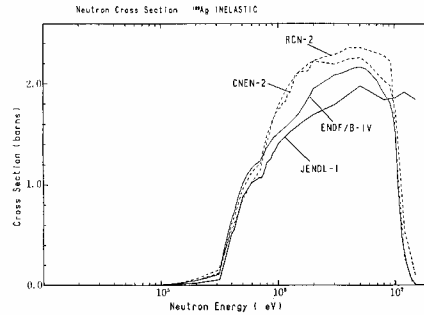


Fig. 3.13.3 Inelastic scattering cross sections of ¹⁰⁹Ag.

Fig. 1 Comparison of JENDL-1 capture and inelastic scattering cross sections for Tc-99 and Ag-109 with the other evaluation and experimental data.[Ref. 9]

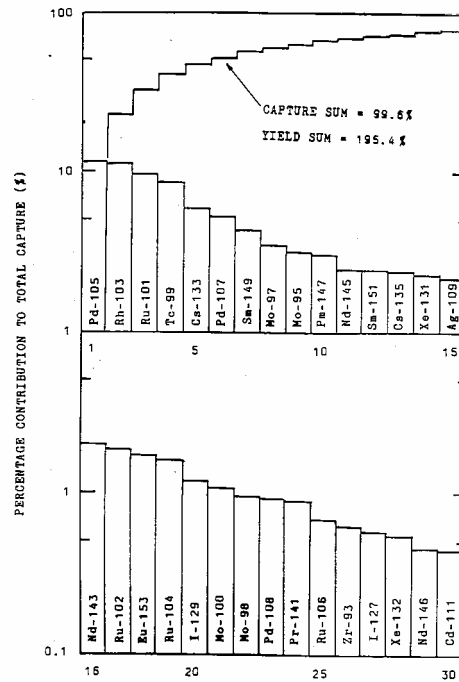


Fig. 2 30 keV neutron capture contributions of most important 30 nuclides. [Ref. 14]

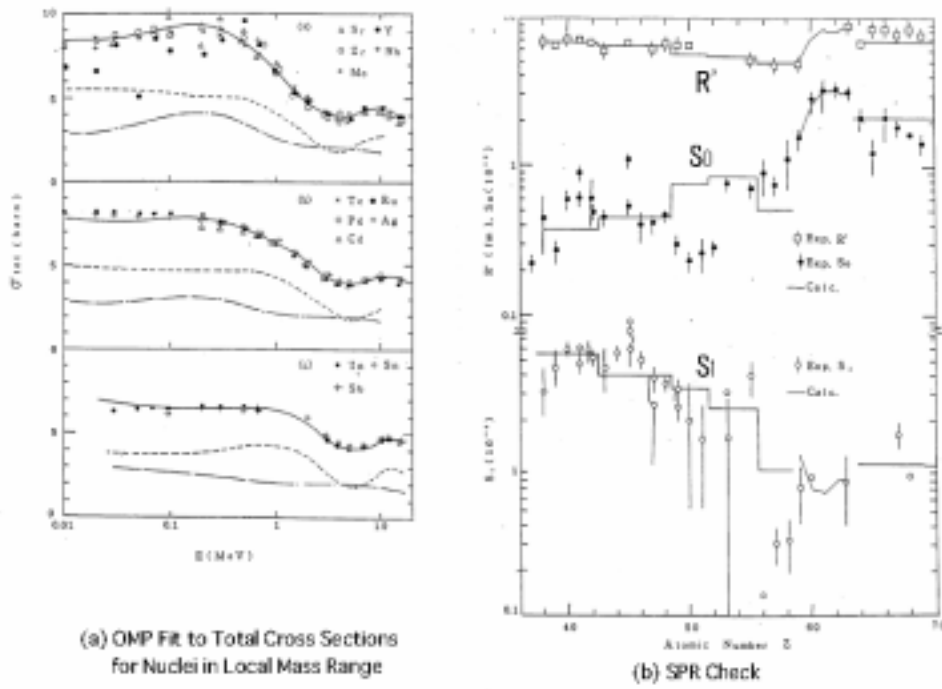


Fig. 3 Determination of optical model parameters with SPRT method[Ref.17]

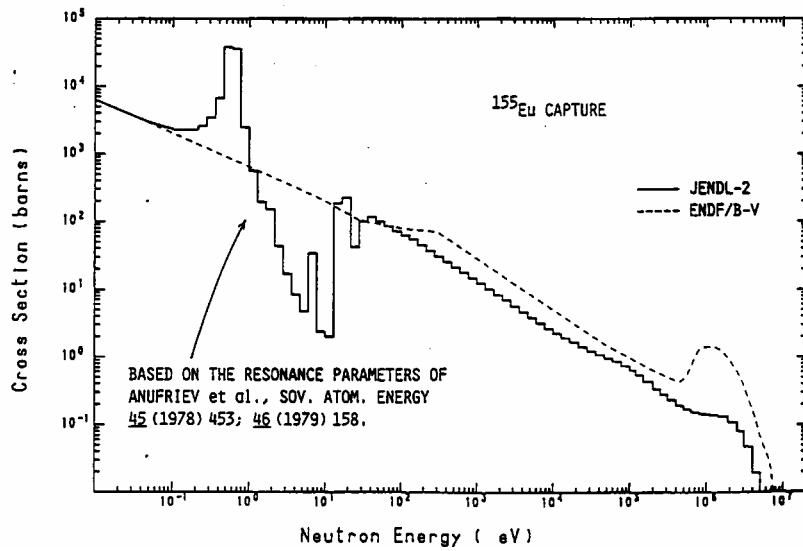
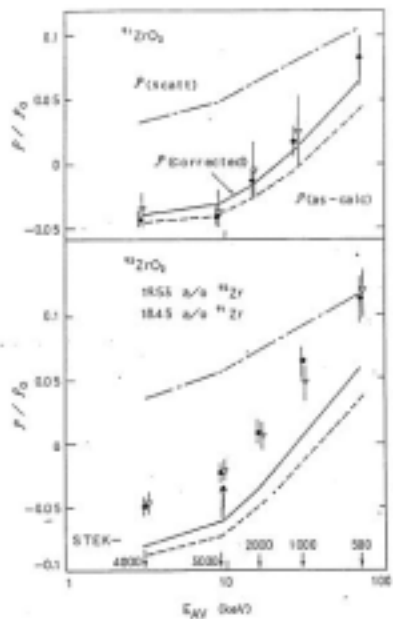
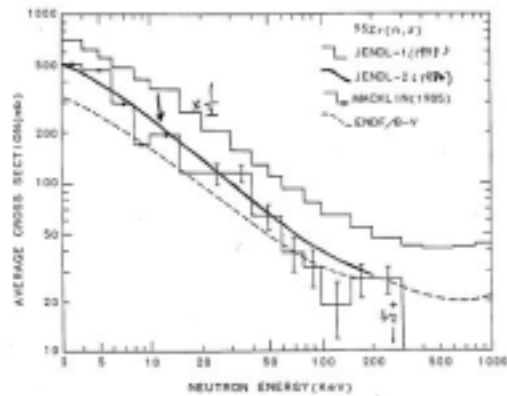


Fig. 4 Comparison of capture cross section for Eu-155[Ref. 14]



(a) Reactivity Worth of Zr-91 and Zr-93



(b) Capture Cross Section of Zr-93

Fig. 5 Integral test results and evaluation of capture crss sections of Zr-93.[Ref.14]

(a) Calculated reactivity worth with JENDL-1 was corrected for oxygen contributoin. Agreement is good for Zr-91 while systematic overestimation of capture contribution is observed for Zr-93.

(b) JENDL-2 was evaluated by reducing JENDL-1 by a factor of 2 and is agree with the Macklin's data that were reported after JENDL-2.

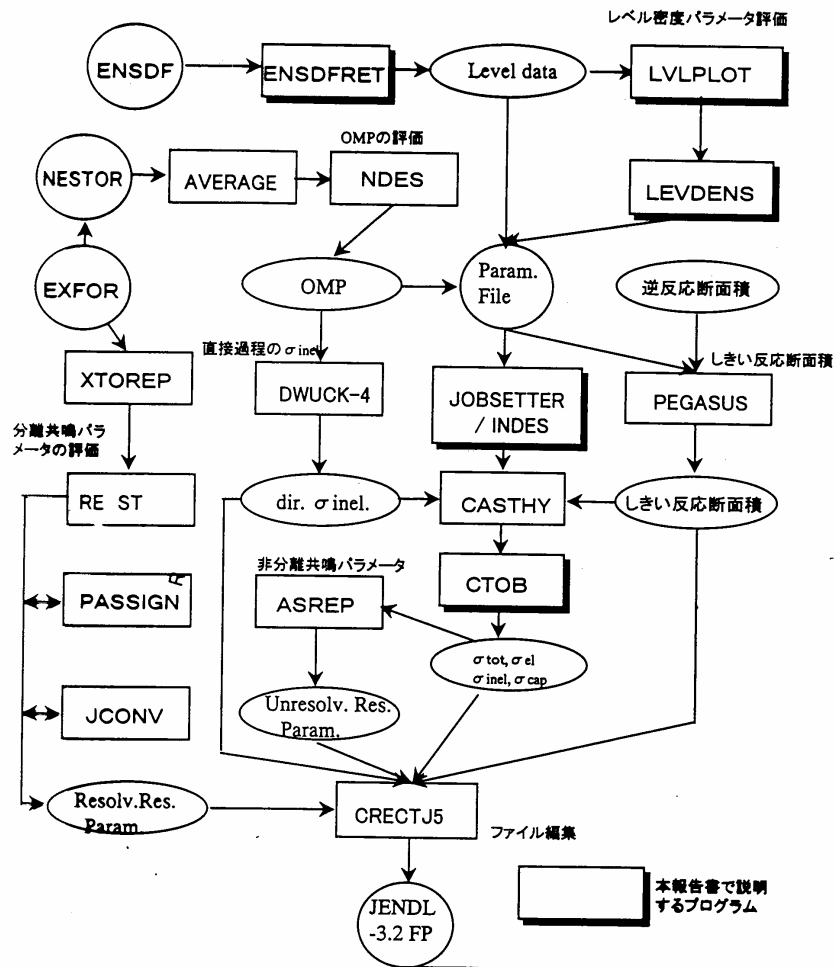


Fig. 6 Evaluation scheme[Re. 24]

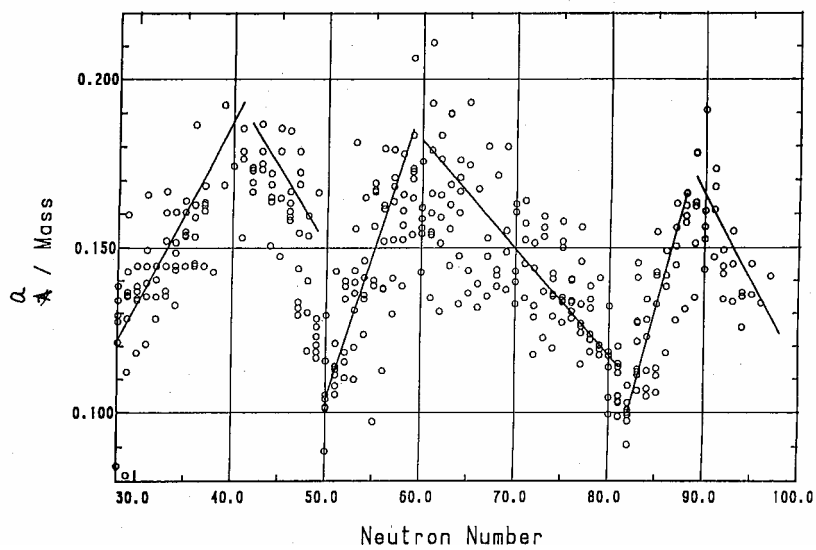


Fig. 7 New systematics of level density parameter, a . [Ref. 29]

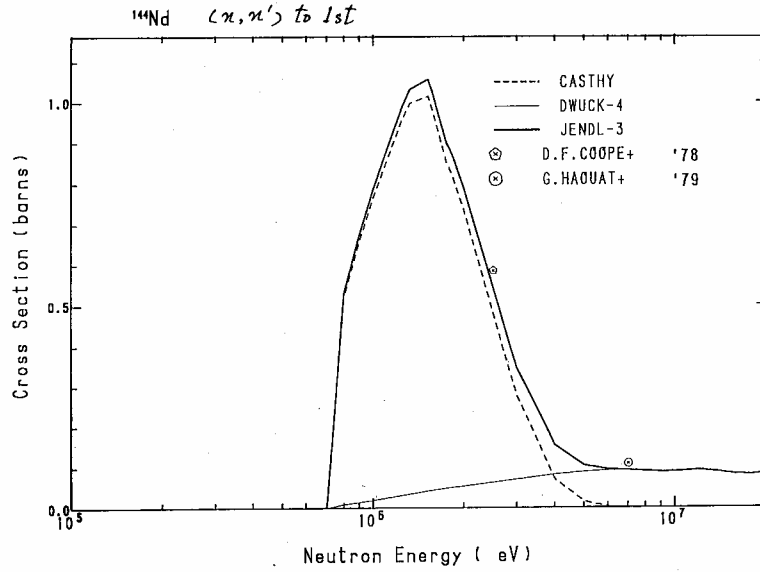


Fig. 8 Comparison of excitation function of inelastic scattering to the first excited state of Nd-144. [Ref. 29]

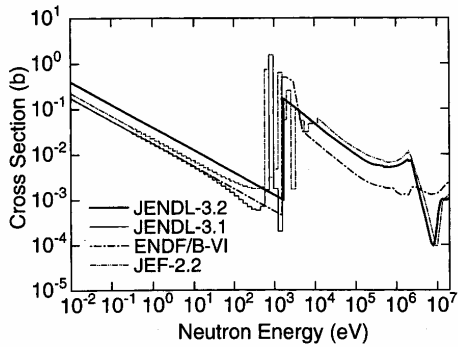


Fig. 1 Capture cross section of ^{137}Cs

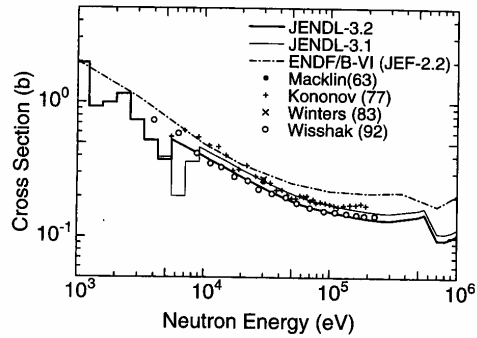


Fig. 3 Capture cross section of ^{148}Sm

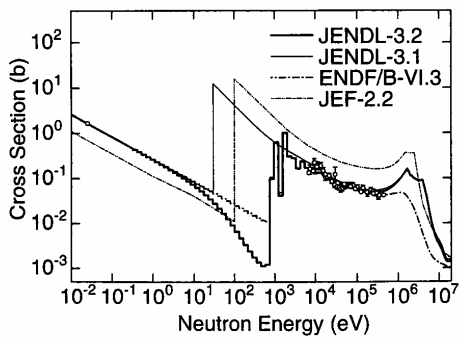


Fig. 2 Capture cross section of ^{144}Sm

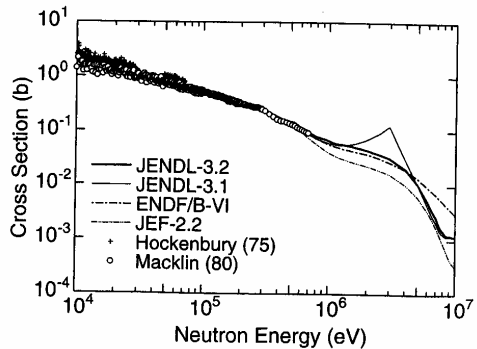


Fig. 4 Capture cross section of ^{101}Ru

Fig. 9 Typical results of evaluated capture cross sections for JENDL-3.2[Ref. 31]

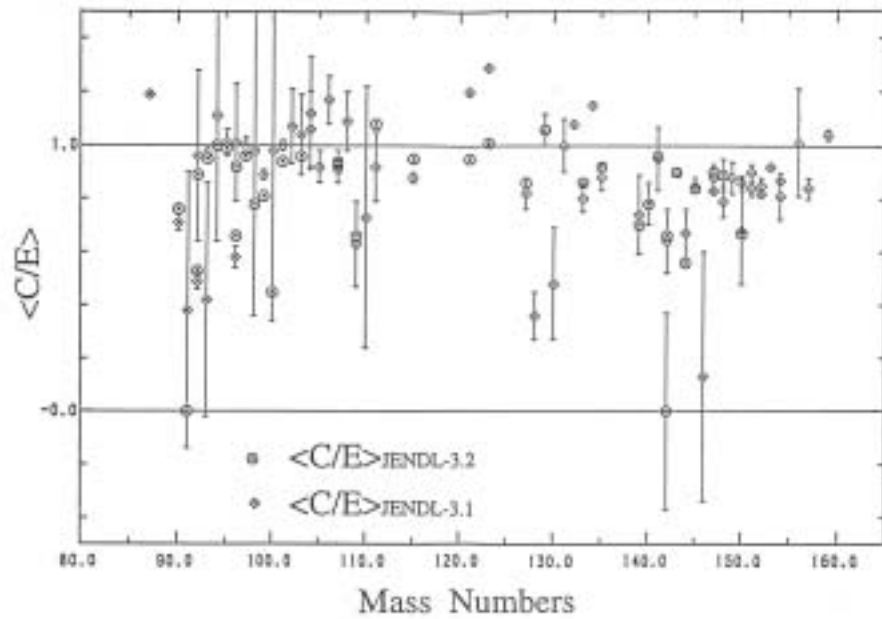


Fig. 10 Comparison of C/E values of sample reactivity worth measured at the STEK Experiments analyzed with JENDL-3.1 and -3.2. [Ref. 33]

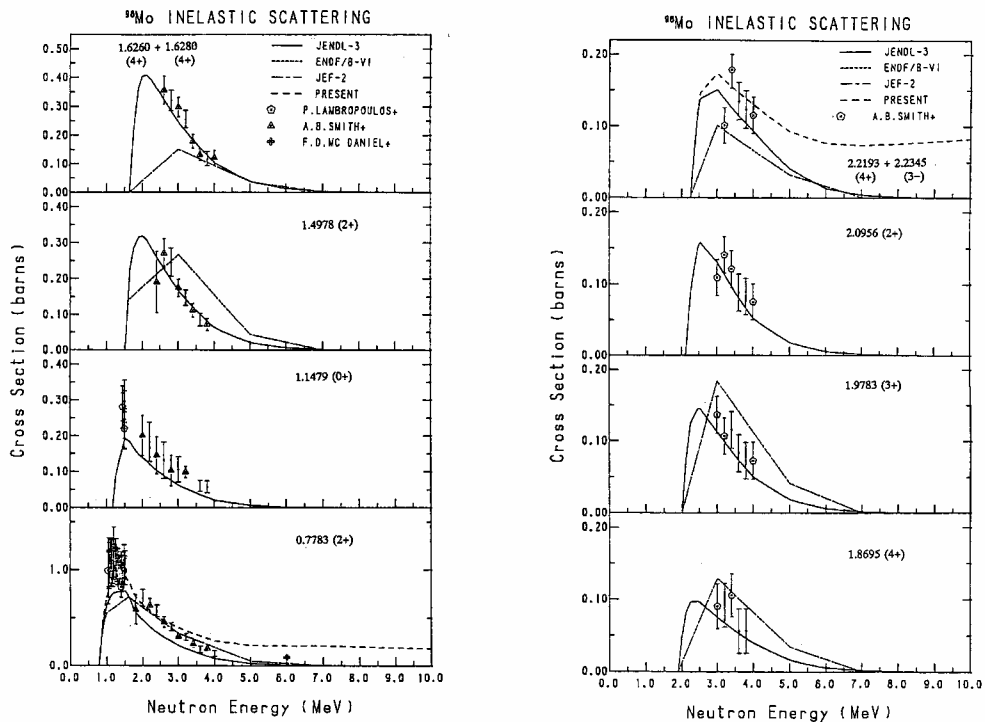


Fig. 11 Comparison of evaluated level excitation functions for Mo-96 with the experimental data. [Ref. 37] PRESENT is calculated with the DWUCK-4 code.

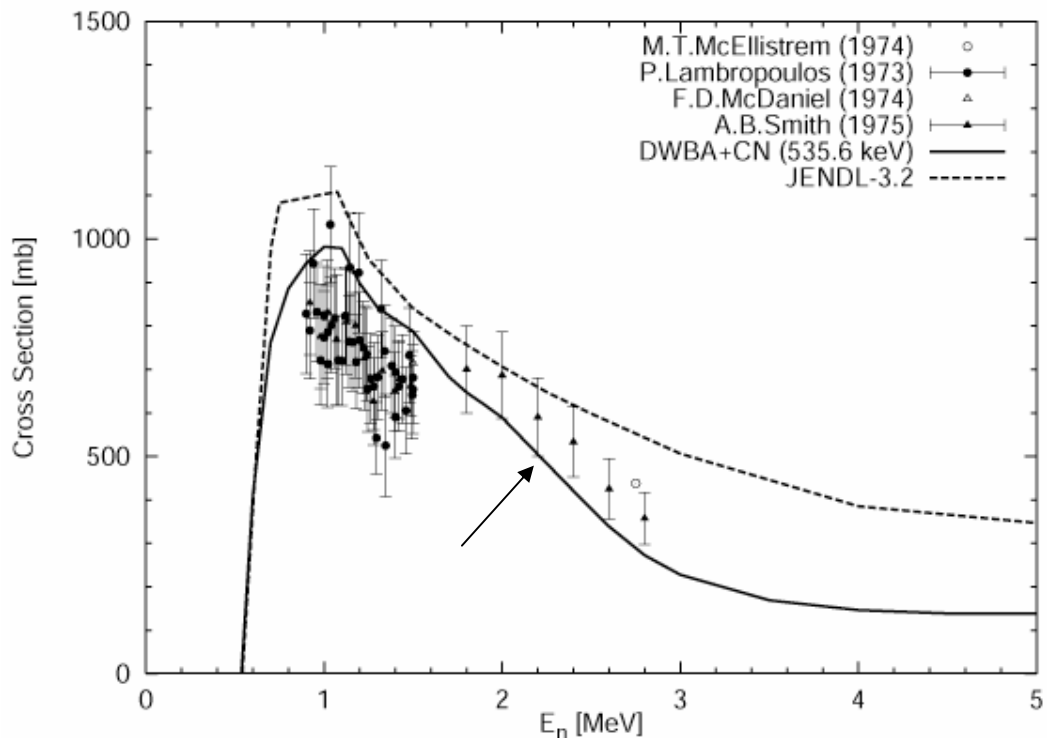


Fig. 12 Inelastic scattering cross section for Mo-100.[Ref. 38]

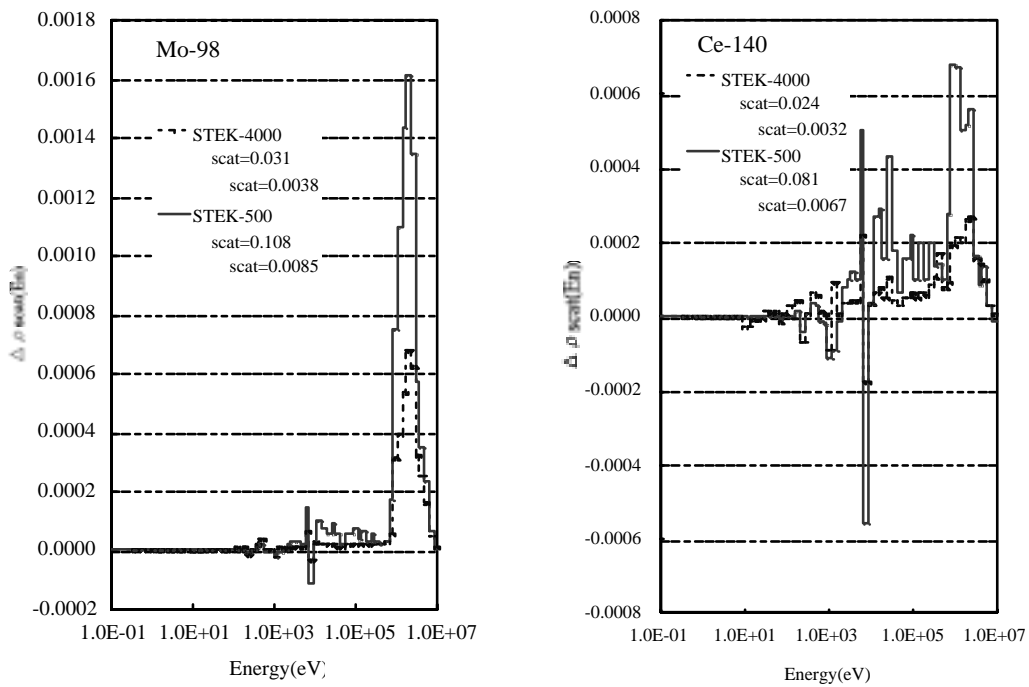


Fig. 13 Sensitivity profile of Mo-98 and Ce-140 against adjoint spectrum difference[Ref. 43]