

CENDL-3.2: The new version of Chinese general purpose evaluated nuclear data library

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Abstract. A new version of Chinese Evaluated Nuclear Data Library, namely CENDL-3.2, has been completed under the joint efforts of CENDL working group. This library is constructed with the general purpose to provide high-quality nuclear data for the modern nuclear science and engineering. 272 nuclides from light to heavy are covered in CENDL-3.2 in total and the data for 134 nuclides are new or updated evaluations in energy region of 10^{-5} eV-20 MeV. The data of most of the key nuclides in nuclear application like U, Pu, Th, Fe et al. have been revised and improved, and various evaluation techniques have been developed to produce the nuclear data with good quality. Moreover, model dependent covariances data for main reaction cross sections are added for 70 fission product nuclides. To assess the accuracy of CENDL-3.2 in application, the data have been tested with the criticality and shielding benchmarks collected in ENDITS-1.0.

1 Introduction

Motivated by fulfilling the increasing requirement of users from diversified nuclear applications, the CENDL project has been initiated under the joint collaboration of CENDL working group, namely China Nuclear Data Center (CNDC) and the Chinese Nuclear Data Cooperation Network (CNDCN) since 1970s. Based on the collaboration of measurements and evaluations, a series versions of CENDL including CENDL-1.0 (1985), CENDL-2.0 (1993) [1], CENDL-3.0 (2000) [2] and CENDL-3.1 (2009) [3] had been released, which to provide evaluated neutron reaction data from light to heavy nuclides in the past. After CENDL-3.1, more advanced nuclear reaction models, measurements, evaluation approaches, visualization systems for evaluation, and the benchmark testing tools et al. have been developed in the latest CENDL project to improve the new evaluated data, and a new library for neutron data, namely CENDL-3.2 is formed. The total nuclides in CENDL have been increased from the first 37 nuclides in CENDL-1.0 to the current 272 nuclides in CENDL-3.2. Through the criticality and shielding benchmark testing with ENDITS-1.0 [4], CENDL-3.2 was proved to make the obvious progress in application comparing to CENDL-3.1.

The current methodologies applied in CENDL-3.2 are gradually set up through the joint contributions from CNDC and more than 10 Chinese universities and institutions in the past ten years. Meanwhile, CENDL-3.2 also benefits from the international collaborative such as NRDC network, IAEA/CRPs, OECD/WPEC Subgroups et al.. In the evaluation process, according to the status of

available experimental data, including the recently measurements performed by CNDCN, various methods based on the phenomenological and microscopic theoretical models and some empirical approaches are applied to deal with different cases from the light nuclides to the heavy nuclides. Among them, several highlight researches are focused after CENDL-3.2b0 reported in ND2016 [5] including the microscopic nucleon-nucleon interaction for the n-n and n-p data, the Faddeev-AGS few body calculations for light nuclides, the theoretical nuclear reaction system for fission products and actinides with MINUIT [6], and the deterministic least square approach for the model-dependent covariance of fission product nuclei and so on.

In this paper, the major achievement of CENDL-3.2 are overall depicted in Sec.2, where the features of evaluations for each mass region and the relevant applied methodologies are briefly discussed at the same time. Then, the benchmark and validation for CENDL-3.2 are introduced in Sec.3 to validate its reliability. Finally, the conclusion and perspective are presented in Sec.4.

2 CENDL-3.2 and Methodologies

The main part of CENDL is the neutron reaction data. The current CENDL-3.2 is developed based on the reported intermediate version CENDL-3.2b0, which was systematically introduced during ND2016 [5]. After then, the total number of nuclides in CENDL-3.2 is enhanced from 250 in CENDL-3.2b0 to 272 in CENDL-3.2, as shown in Table 1, several nuclides are re-evaluated and the

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covariance files of fission product nuclides are systematically added in this version.

Table 1. Nuclides list and major updates for CENDL-3.2

Newly Evaluated and Partly Updated (135 Nuclides)
<p>Newly Evaluated (58 Nuclides): n-1, H-1, Na-23, Al-27, S-32, S-33, S-34, S-36, Ca-40, Fe-56, Ni-58, Zn-64, Zn-66, Zn-67, Zn-68, Zn-70, Se-74, Se-76, Se-77, Se-78, Se-79, Se-80, Se-82, Kr-87, Kr-88, Mo-93, Mo-99, Sn-126, Sn-128, Sb-124, Sb-127, I-130, I-131, Xe-123, Xe-124b, Xe-129, Xe-131, Xe-132b, Xe-133, Xe-134b, Xe-135b, Xe-136, La-139b, Ce-140, Ce-141b, Ce-142, Ce-144b, Ho-165, W-180, W-182, W-183, W-184, W-186, U-236, U-240, Np-236, Pu-238, Am-241.</p>
<p>Partly Updated (77 Nuclides): H-2, Li-7, Ti-48, Ga-69^a, Ga-71^a, Ge-71^a, Ge-73^a, Ge-74^a, Ge-75^a, Ge-76^a, Ge-77^a, Ge-78^a, As-75^a, As-77^a, As-79^a, Sr-89^a, Y-89^a, Y-91^a, Zr-93^a, Zr-95^a, Nb-93, Nb-95^a, Tc-99^a, Ru-99^a, Ru-100^a, Ru-101^a, Ru-103^a, Ru-104^a, Ru-105^a, Rh-103^a, Rh-105^a, Pd-105^a, Pd-108^a, Cd-113^a, Sb-121^a, Sb-125^a, I-127^a, I-129^a, I-135^a, Cs-133^a, Cs-135^a, Cs-137^a, Ba-130^a, Ba-134^a, Ba-135^a, Ba-136^a, Ba-137^a, Ba-138^a, Pr-141^a, Nd-143^a, Nd-145^a, Nd-146^a, Nd-148^a, Pm-147^a, Pm-148^a, Pm-149^a, Sm-150^a, Sm-151^a, Eu-151^a, Eu-153^a, Eu-155^a, Gd-154^a, Gd-155^a, Gd-156^a, Gd-157^a, Gd-158^a, Gd-160^a, Th-232, U-233, U-235^b, U-237, U-238^b, U-239, Np-237, Np-239, Pu-240, Pu-241^b.</p>
<p>Inherited from CENDL-3.1 (137 Nuclides): H-3, He-3, He-4, Li-6, Be-9, B-10, B-11, C-12, N-14, O-16, F-19, Mg-24, Mg-25, Mg-26, Si-28, Si-29, Si-30, P-31, Cl-0, K-0, Ca-0, Ti-46, Ti-47, Ti-49, Ti-50, V-0, Cr-50, Cr-52, Cr-53, Cr-54, Mn-55, Fe-54, Fe-57, Fe-58, Co-59, Ni-60, Ni-61, Ni-62, Ni-64, Cu-0, Cu-63, Cu-65, Ge-0, Ge-70, Ge-72, Kr-83, Kr-84, Kr-85, Kr-86, Rb-85, Rb-87, Sr-88, Sr-90, Zr-90, Zr-91, Zr-92, Zr-94, Zr-96, Mo-92, Mo-94, Mo-95, Mo-96, Mo-97, Mo-98, Mo-100, Ru-102, Ag-0, Ag-107, Ag-109, Cd-0, In-113, In-115, Sn-0, Sn-112, Sn-114, Sn-115, Sn-116, Sn-117, Sn-118, Sn-119, Sn-120, Sn-122, Sn-124, Sb-123, Te-130, Cs-134, Ba-132, Ce-136, Ce-138, Nd-142, Nd-144, Nd-147, Nd-150, Pm-148m, Sm-144, Sm-147, Sm-148, Sm-149, Sm-152, Sm-154, Eu-154, Gd-152, Dy-164, Hf-174, Hf-176, Hf-177, Hf-178, Hf-179, Hf-180, Ta-181, Au-197, Hg-0, Tl-0, Pb-204, Pb-206, Pb-207, Pb-208, Bi-209, U-232, U-234, U-241, Np-238, Pu-236, Pu-237, Pu-239, Pu-242, Pu-243, Pu-244, Pu-245, Pu-246, Am-240, Am-242, Am-242m, Am-243, Am-244, Bk-249, Cf-249.</p>

- a. Covariance added.
- b. Beta-delayed fission gamma spectrum (MT=460) added.

2.1 Light nuclides

In the light mass region, the final accepted modifications in CENDL-3.2 are the new evaluations for n, ¹H. The high-precise microscopic nucleon-nucleon (N-N) interaction CD-Bonn [7] is selected to present the new n-n and n-p scattering data for CENDL-3.2. The charge independent breaking (CIB) and the charge symmetry breaking (CSB) are considered seriously in CD-Bonn interaction, and it is shown that both n-n and n-p scattering cross sections based

on the current study are slightly larger than the data in ENDF/B-VIII.0 [8], about 1 barn below the incident neutron energy $E_n \sim 1$ MeV, as shown in Fig. 1. The update for n-p is shown in Fig. 2, and similar deviation can also be observed in the n-p system.

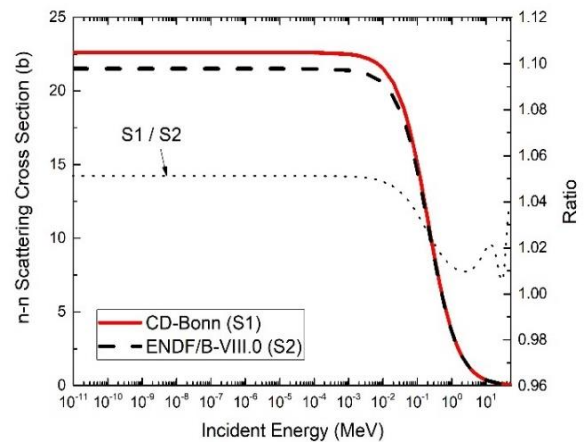


Fig. 1. The evaluated results for neutron-neutron scattering data based on the CD-Bonn interaction.

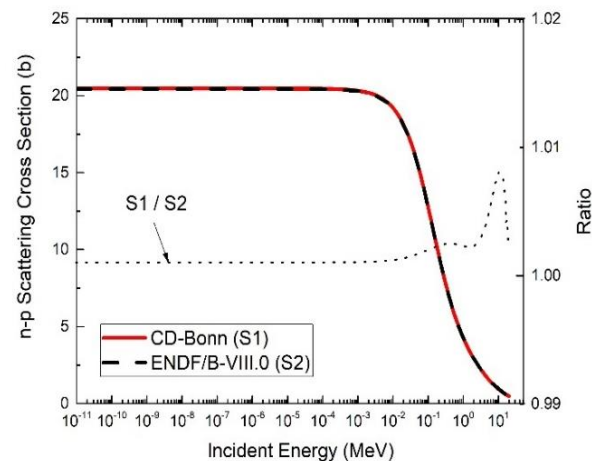


Fig. 2. The evaluated results for neutron-proton scattering data based on the CD-Bonn interaction.

Addition to the scattering cross sections of n-n and n-p, the new evaluations for D and ^{6,7}Li are also carried out for CENDL-3.2. As for the n+D system, the wave packet continuum discretization [9] is involved in solving the Faddeev-AGS equation in the study of three-body scattering theory, and the work is carried out under the collaborations between Beihang University and Moscow State University. In Fig. 3, the derived double differential cross sections for neutron emission at $E_n = 14.1$ MeV for n+D reaction are shown, and the results reproduce the experimental data very well.

As for the neutron data of Li to F, the combined scheme is designed to generate the complete neutron data for light nuclei, which is based on FDRR code with the full diagonal R-matrix approach and the nuclear reaction code system LUNF with the nuclear statistical model [10]. The flow diagram in FDRR is shown in Fig. 4, and the calculated angular distributions for n+⁶Li elastic scattering reaction cross sections are shown in Fig. 5, and the satisfying agreements between the experimental data and the calculated results are shown.

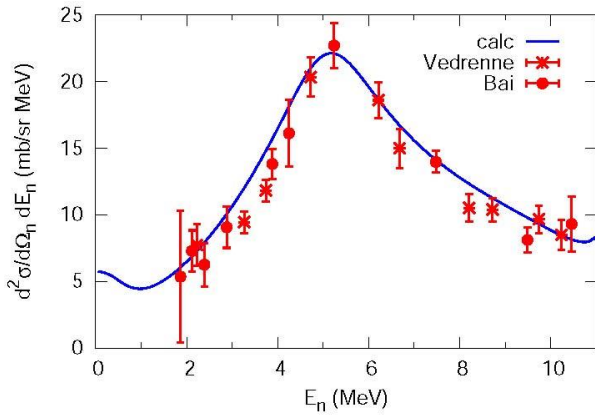


Fig. 3. The comparison between the calculated double differential cross sections and experimental data (Vedrenne [11] and Bai [12]), the incident neutron energy $E_n = 14.1$ MeV and the secondary neutron emission angle is 15° .

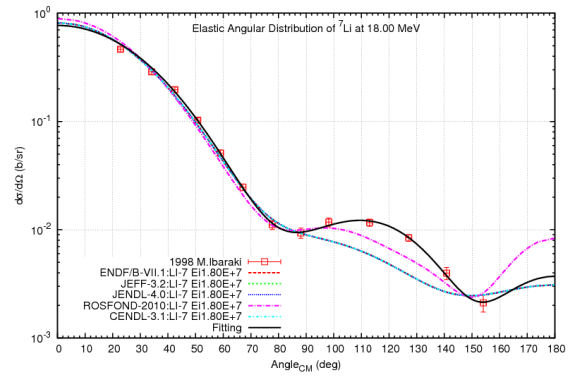


Fig. 6. The updated angular distribution of the $n+{}^7\text{Li}$ elastic scattering reactions at $E_n = 18$ MeV. The solid lines for the Legendre fittings, and the dots are experiment data in EXFOR [13].

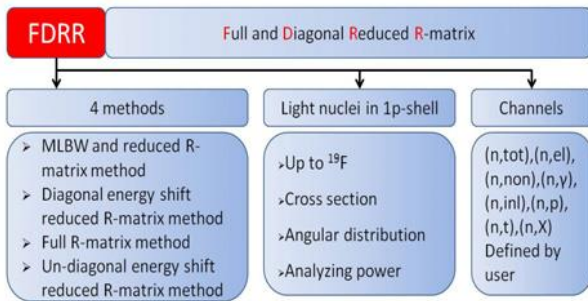


Fig. 4. The current flow diagram of the R-Matrix code FDRR.

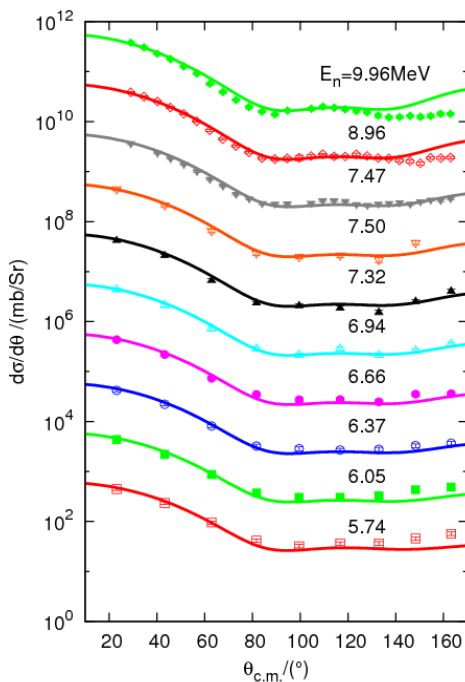


Fig. 5. The angular distributions of the $n+{}^6\text{Li}$ elastic scattering reactions at $E_n = 5.74, 6.05, 6.37, 6.66, 7.32, 7.5, 7.47, 8.96, 9.96$ MeV. The solid lines for the R-matrix calculations, and the dots are experiment data in EXFOR [13].

Moreover, the angular distributions of $n+{}^7\text{Li}$ elastic scattering are also updated based on the experimental data with the new Legendre fittings in CENDL-3.2. The data of $E_n = 18$ MeV sampled in Fig. 6 shows the improvement.

2.2 Medium-heavy nuclides

In this mass region, the UNF reaction code [14] is used to calculate the nuclear reaction data for the medium-heavy nuclides (structural materials and fission product nuclides), and the experimental data evaluation is performed to provide necessary guidance to the theoretical calculation. The data of Na, Al, S, Ca, Fe, and W isotopes have been newly evaluated and updated as shown in Table 1. Regards to these nuclides, the evaluation for ${}^{56}\text{Fe}$ attracts more attention internationally, especially to the inelastic scattering cross section. To obtain the reliable data, many ways were applied to clarify the discrepancy in the energy range between 9-11 MeV. The current ${}^{56}\text{Fe}(n,\text{inl})$ cross section evaluation in smooth region for CENDL-3.2 are based on the experimental data recommended by Jing Qian in the CIELO project [15]. The gamma-ray production cross sections provide a method to gain experimental information of ${}^{56}\text{Fe}(n,\text{inl})$. To solve the problem of under prediction of neutron leakage in the iron shielding benchmark, the experimental data of ${}^{56}\text{Fe}(n,\text{inl})$ 847keV gamma production cross sections have been evaluated and a curve for ${}^{56}\text{Fe}(n,\text{inl})$ reaction cross section is obtained (in Fig. 7), which is based on the corrections to Nelson's data (2004) around 14 MeV [16].

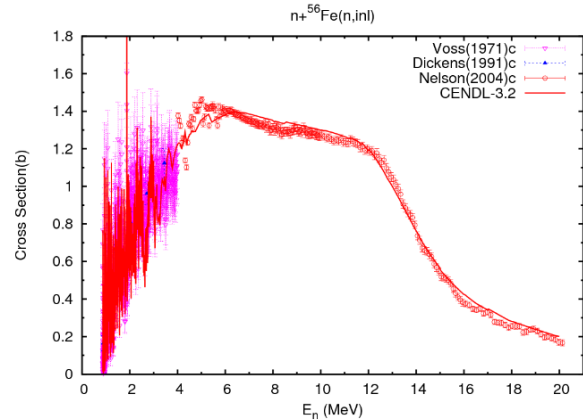


Fig. 7. The comparison between the ${}^{56}\text{Fe}(n,\text{inl})$ reaction cross section in CENDL-3.2 and experimental data [13].

Moreover, the re-evaluation of ${}^{56}\text{Fe}(n,\text{inl})$ reaction cross section is also performed to satisfy the requirement

from the design of the sodium-cooled fast reactor, CFR-600, in Fujian Province, China. As a result, the experimental data and the recommended results in CENDL-3.2 are compared in Fig.7, and significant improvement of validation results has been obtained with the 70cm dia. IPPE iron sphere and the LLNL pulsed iron sphere as shown in Fig. 8.

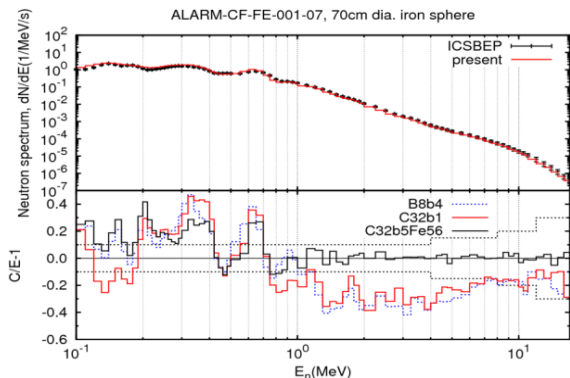


Fig. 8. The comparison between the calculated neutron spectrum with the new evaluated ^{56}Fe data and experimental data from the ALARM-CF-FE-001-07, 70cm dia. Iron sphere.

To exhibit the evaluations for other structure nuclides, parts of the main updated data for other nuclides are listed in Figs. 9-11 and compared with the experimental data and other evaluated data. It is proved that the new data in CENDL-3.2 can coincide with most of the experiment data and the recommended curves are reliable in physics.

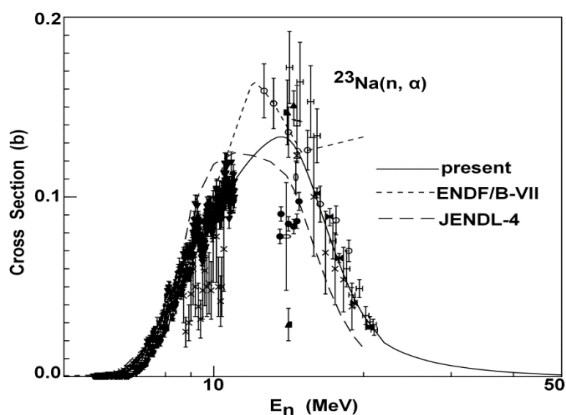


Fig. 9. The comparison of CENDL-3.2 (solid line) and other evaluated (dashed line) for $^{23}\text{Na}(n, \alpha)$ cross section and the available experimental data [13].

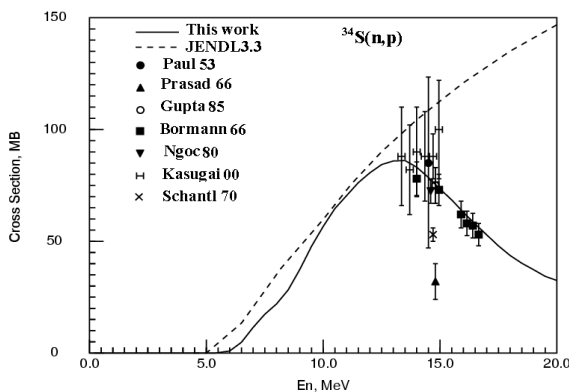


Fig. 10. The comparison of CENDL-3.2 (solid line) and other evaluated (solid line) for $^{34}\text{S}(n, p)$ cross section and the available experimental data [13].

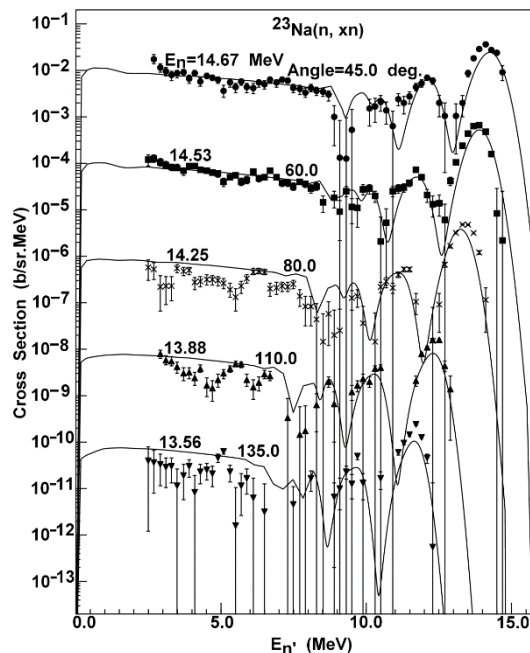


Fig. 11. The comparison of CENDL-3.2 (solid line) for the double differential cross sections of $^{23}\text{Na}(n, xn)$ and the available experimental data [13].

The second major improvement in this mass region is focused on the fission product nuclides. Most of the previous evaluations for fission product nuclides in CENDL-3.0 were obtained with the code SUNF [17], which is an intermediate version for modelling of the product nuclides in the 1990's at CNDC and the data file for double differential cross sections for the secondary particle emission (MF=6) are omitted. In order to add MF-6 file and covariance data MF-33 file in the complete set of neutron data for fission product nuclides, an evaluation project was carried out systematically to handle this problem, the main developed source codes in the evaluation system are described in Table 2. By adopting the minimization tool MINUIT in the system, reaction parameters in UNF are optimized, such as the parameter of the level density, pairing interaction and giant dipole resonance of (n, γ) channel. The ^{147}Pm is sampled in Fig. 12 to illustrate the current data of fission product nuclides in CENDL-3.2 under the optimized calculation system, where the solid line is the cross sections calculated with the new parameters. For the (n, n_1) and (n, n_2) channel, the reasonable cross sections between 8 and 10 MeV region were obtained with the new parameters.

In addition, it is reported that the covariance evaluation method has been developed at CNDC. In the released CENDL-3.2, the covariance file of cross sections (MF=33) for the main nuclear reactions including (n, total) , $(n, \text{elastic})$, (n, γ) , $(n, \text{inelastic})$, (n, p) , $(n, 2n)$ and so on are supplemented to 70 fission product nuclides, as shown in Table 1. The current covariance evaluation methods are systematically established through applying the generalized model dependent evaluations in the structure nuclides and smooth energy regions, the data files are output in the NI and NC format types to generate the covariance data for different reactions to distinguish the data evaluated in terms of other data. Moreover, abundant of measurements for nuclear reaction cross sections are

indirectly considered in the covariance evaluation via the parameter covariance. The model parameter sensitivities of the optical model, equilibrium and pre-equilibrium model, direct reaction model are estimated according to the non-model dependent covariance matrices from the experimental data of the 70 fission product nuclides. As a result, the averaged evaluated uncertainties for each cross sections in CENDL-3.2 are about 10% for (n,total), 30% for (n, γ), 20% for (n,inelastic), 20% for (n,2n) and 80% - hundred percent for the charged particle emission reactions.

Table 2. The source codes in the FP evaluation system.

Source scripts	Functions
sunf2unf	Convert inputs of SUNF to UNF
Batchcal	Batch production for UNF inputs
batchmincard	Auto-produce inputs SEMAW.in, DPPMI.in, Min.in, sys.dat, exp
Correctmin	Correct the energy margin of min.in
get14MevCSInl	Produce the direct reaction cross section
batchmincard14	Adjust DWUCK para. to fit 14 MeV
NDPlot	Plot the figures for 10 reactions

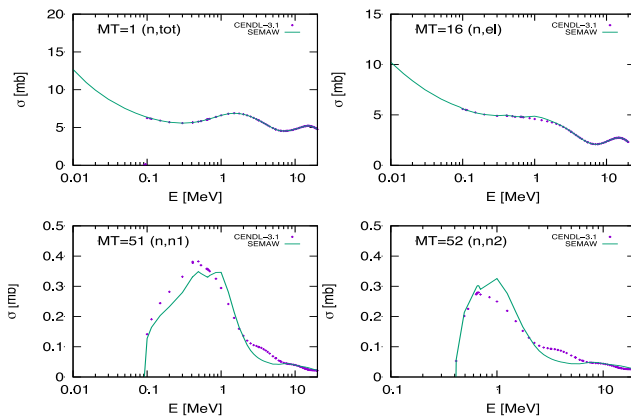


Fig. 12. The comparison of CENDL-3.1 (points) and CENDL-3.2 (line) for the cross sections of n+¹⁴⁷Pm reaction.

2.3. Fission nuclides

In this mass region, the important actinides U, Pu, Th, Np, Am are updated based on the non-model dependent systematics in the experimental data evaluation and the theoretical calculation based on the FUNF code [18].

The important modifications are performed to ²³⁵U to obtain better benchmark testing results around $E_n = 3$ MeV. Firstly, the nubar and resonance parameters of ²³⁵U in CENDL-3.2 were optimized to reproduce the thermal quantities of the IAEA 2006 standard [19], which improves the prediction of k_{eff} for the HMT system. Secondly, the (n, γ) cross sections were revised based on the available experimental $\alpha = \sigma_\gamma/\sigma_f$ value and the (n,f) cross sections recommended in IAEA 2006 standard cross sections and re-evaluated α values. Benchmark testing with the selected HMF, IMF and HMI cores show that the predictions of k_{eff} get closer to 1 than before. The comparison between the evaluated α values and the experimental data are shown in Fig. 13, and the benchmark testing results using the modified ²³⁵U data are compared in Fig. 14.

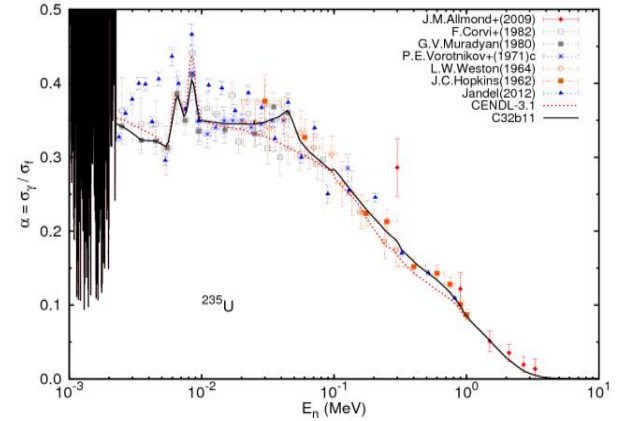


Fig. 13. The comparison between the evaluated α values and the experimental data in EXFOR/CSISRS [20].

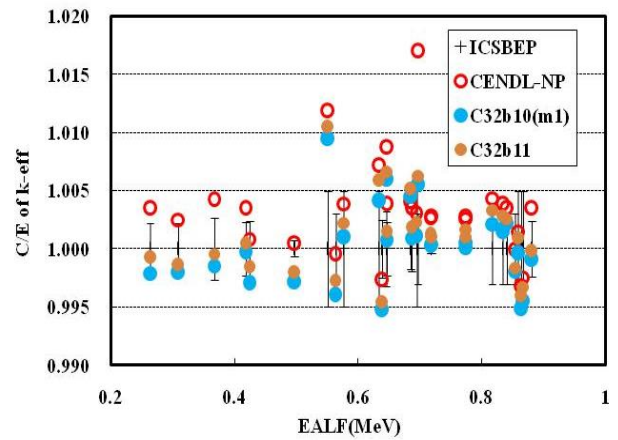


Fig. 14. The comparison of C/E of k_{eff} between ICSBEP, CENDL-NP, CENDL-3.2b10 and CENDL-3.2.

In the other hand, the big efforts have been dedicated to improve the data for other actinides based on CENDL-3.1. Fig. 15 shows the modification of ²³³U (n, inl) cross sections in CENDL-3.2 based on the systematics and benchmark testing. In Fig. 16, the delayed fission neutron multiplicity data of ²³³U is sampled to illuminate the updates according to the experimental data. The evaluations for ²⁴¹Am(n,2n) and (n, f) cross sections are plotted in Figs. 17-18, and the results agree well with the concerned experimental data.

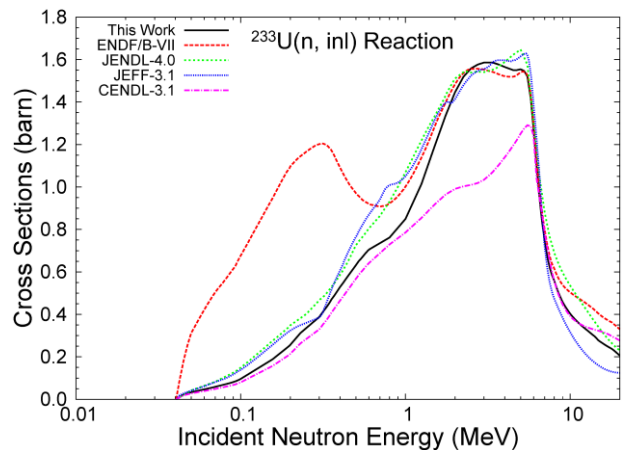


Fig. 15. The modification for ²³³U(n,inl) cross sections in CENDL-3.2, and the comparison to other evaluated data.

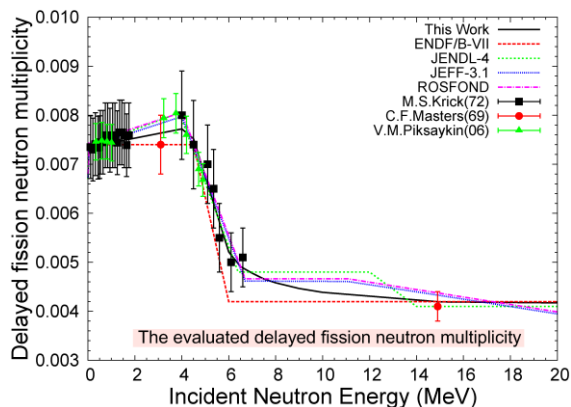


Fig. 16. The comparison of the modified delayed fission neutron multiplicity for ^{233}U in CENDL-3.2 and the other evaluated and the experimental data [13].

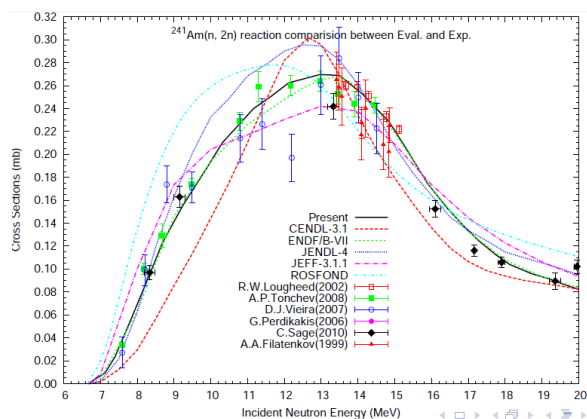


Fig. 17. The comparison of the updated $^{241}\text{Am}(n,2n)$ in CENDL-3.2 and the other evaluated and the experimental data [13].

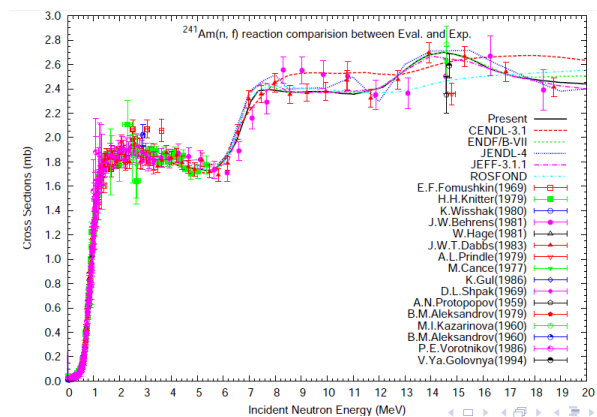


Fig. 18. The comparison of the updated $^{241}\text{Am}(n,f)$ in CENDL-3.2 and the other evaluated and the experimental data.

3 Validations and Application

In order to verify the physical rationality, systematic comparisons between CENDL-3.2 and other major evaluated libraries (e.g. ENDF, JENDL, BROND, JEFF and TENDL) as well as available experimental data have been implemented. Moreover, the benchmark testing of CENDL-3.2 was performed with ENDITS-1.0, an integrated benchmark testing system including 1261 criticality benchmark configurations. Figs. 19-22 illustrate the benchmark testing results for CENDL-3.2 in various systems, as well as comparisons with ENDF/B-VIII.0 [8],

JENDL-4.0 [21] and JEFF-3.2 [22]. As shown in Table 3, the χ^2 value implies that CENDL-3.2 has a potential remarkable improvement of predictions for ^{235}U and Pu systems.

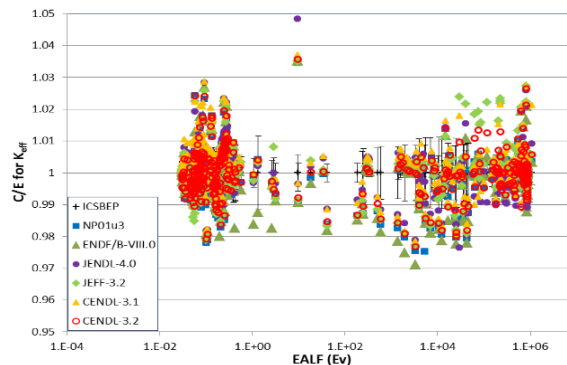


Fig. 19. Results for HEU systems

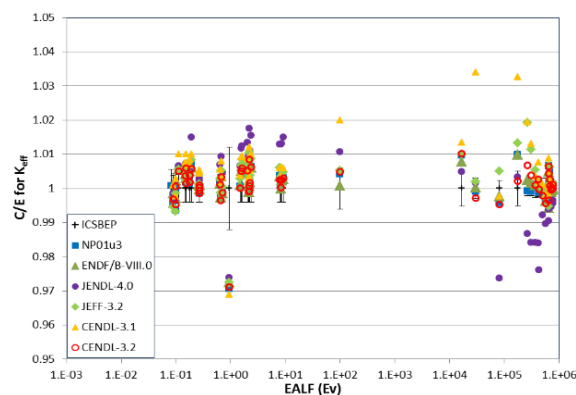


Fig. 20. Results for IEU systems

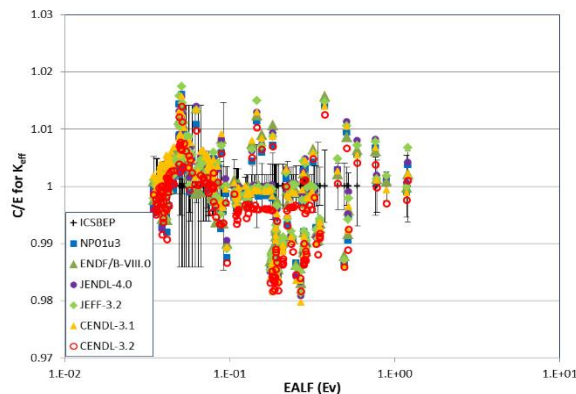


Fig. 21. Results for LEU systems

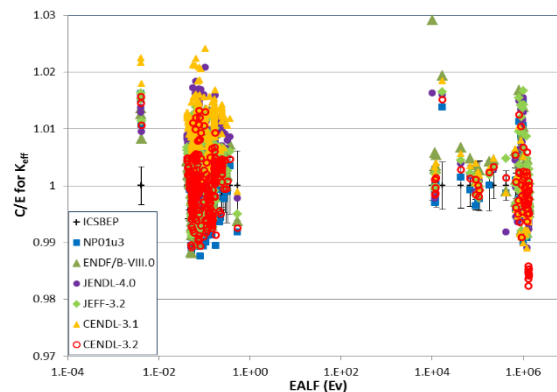


Fig. 22. Results for Pu systems

Table 3. The comparison of the benchmark testing for CENDL-3.2 and CENDL-3.1.

Type	Cores	Quantity	CENDL-3.2	CENDL-3.1
U-235	698	C/E-1(pcm)	-13	197
		STDEV	828	912
		χ^2	16.94	31.91
U-Pu	7	C/E-1(pcm)	155	-36
		STDEV	277	285
		χ^2	20.40	11.89
Pu	388	C/E-1(pcm)	27	729
		STDEV	511	788
		χ^2	2.80	8.90
U-233	165	C/E-1(pcm)	-449	-36
		STDEV	1206	1196
		χ^2	5.18	6.52
All	1261	C/E-1(pcm)	-58	327
		STDEV	821	958
		χ^2	11.03	21.33

4 Conclusion and Perspective

Compared with the previous CENDL libraries, the current CENDL project aims to build a new complete nuclear data library constituted by the nuclear reaction data of neutron and charged particles, photonuclear data, fission yield, decay and activation files. In this paper, the new released CENDL-3.2 for neutron data and the applied methodologies are briefly introduced. As the main output of CENDL project, CENDL-3.2 is built with the general purpose to provide high-quality nuclear data for the modern nuclear science, engineering and nuclear technology etc. The updated evaluation of nuclear reaction data for several key nuclides, such as $^{235,233}\text{U}$, ^{232}Th , ^{56}Fe et al. have been revised and improved. The library was tested with the criticality and shielding benchmarks, better results have been obtained, and used for applications, such as Chinese CEFR, TMSR, CAP1400, ADS, BIRF, JUNA, BISOL projects.

CENDL future will benefit from the issues related to the progress of fundamental nuclear physics, such as the theories for the fission, the few body calculation, the microscopic studies for light nuclides and unstable neutron-rich nuclides, and the international nuclear data measurements, evaluation etc. Deeper and further international co-operation is highly required in the future.

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