EPJ Web of Conferences 284, 14011 (2023) https://doi.org/10.1051/epjconf/202328414011
ND2022

Deuteron and alpha sub-libraries of JENDL-5

Shinsuke Nakayama[1,*], Osamu Iwamoto[1], and Jean-Christophe Sublet[2]

[1]Nuclear Data Center, Japan Atomic Energy Agency, Tokai, Japan
[2]Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria

Abstract. JENDL-5, the latest version of the Japanese evaluated nuclear data library, includes several sub-libraries to contribute to various applications. In this paper, we outline the evaluation and validation of the deuteron reaction sub-library developed mainly for the design of accelerator-based neutron sources and the alpha-particle reaction sub-library developed mainly for use in the back-end field. As for the deuteron sub-library, the data for ^{6,7}Li, ^{9}Be, and ^{12,13}C from JENDL/DEU-2020 were partially modified and adopted. The data up to 200 MeV for ^{27}Al, ^{63,65}Cu, and ^{93}Nb, which are important as accelerator structural materials, were newly evaluated based on the calculations with the DEURACS code. As for the alpha-particle sub-library, the data up to 15 MeV for 18 light nuclides from Li to Si isotopes were evaluated based on the calculations with the CCONE code, and then only the neutron production cross sections were replaced with the data of JENDL/AN-2005. Validation on neutron yield by Monte Carlo transport simulations was performed for both sub-libraries. As a result, it was confirmed that the simulations based on the sub-libraries showed good agreement with experimental data.

1 Introduction

JENDL-5 is the latest version of the Japanese evaluated nuclear data library released in December 2021 [1]. JENDL-5 has 11 sub-libraries to meet a variety of needs from application areas such as nuclear reactors, shielding design, accelerators, etc. This paper outlines the evaluation and validation of the two sub-libraries of them. One is the deuteron sub-library developed mainly for the design of accelerator-based neutron sources. The other is the alpha-particle sub-library developed mainly for application in the back-end fields.

2 Deuteron sublibrary

As for deuteron nuclear data, we have recently developed JENDL/DEU-2020 [2], a deuteron nuclear data library for Li, Be, and C isotopes up to 200 MeV. This is because intensive neutron sources using (d,xn) reactions on these light elements have been proposed for various applications. As an example of the Monte Carlo transport simulations using JENDL/DEU-2020, Fig.1 shows the double-differential neutron yields from thick carbon target bombarded by a 18-MeV deuteron. The solid and dash-dotted lines represent the simulations with the PHITS code [3] using the ACE files based on JENDL/DEU-2020 and TENDL-2021 [4], respectively. The dashed line shows the results using the nuclear reaction models incorporated in the PHITS code. In this simulation, INCL-4.6 [5] is used to calculate dynamical processes and GEM [6] is used to calculate evaporation processes. These models are the recommended ones in PHITS for deuteron-induced reactions. Experimental data are taken from Ref. [7]. As shown in the figure, the simulations using JENDL/DEU-2020 reproduces the experimental data well.

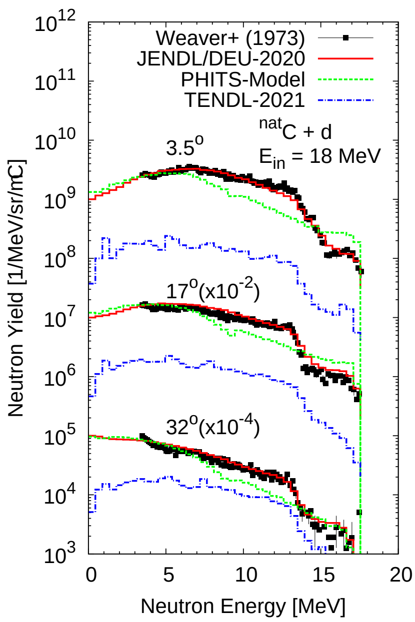

Figure 1. Experimental and simulated double-differential neutron yields from a thick natural carbon target bombarded by a 18-MeV deuteron. The numbers at the top of each plot indicate the emission angles.

*e-mail: nakayama.shinsuke@jaea.go.jp

It is described in Ref. [2] that the transport simulations based on JENDL/DEU-2020 also well reproduce the experimental neutron yield data for combinations of target and incident energy different than in Fig. 1. Therefore, JENDL/DEU-2020 were adopted as the data for ^{6,7}Li, ^{9}Be, and ^{12,13}C in the deuteron sub-library, except for some minor modifications. Some modifications were made to data such as the triton production cross sections on ^{6}Li below 10 MeV, but no change was made to the neutron production data below 50 MeV, which are often used in accelerator-based neutron source design.

Deuteron nuclear data for accelerator structural materials are also important from the perspective of shielding design of accelerator facilities. Therefore, we performed a new evaluation of deuteron nuclear data up to 200 MeV for ^{27}Al, ^{63,65}Cu, and ^{93}Nb. In the evaluation, the DEURACS code [8] was employed. DEURACS is a computational code for deuteron-induced reactions we have developed and it was employed also in the evaluation of JENDL/DEU-2020. Since deuteron is a weakly bound system, it easily breaks up and emits neutron through interaction with other nucleus. Due to this property, it is important to consider the breakup processes in the evaluation of deuteron-induced neutron production data. Moreover, the (d,n) transfer reactions to specific bound states in the residual nuclei contribute significantly to neutron emission, especially at low incident energies. In DEURACS, these reaction processes can be taken into account by means of the theoretical models according to individual reaction processes.

As an example of the validation results, those for the double-differential neutron yields from a thick natural copper target bombarded by a 9-MeV deuteron are shown in Fig. 2. The meaning of each line is the same as in Fig. 1. Experimental data are taken from Ref. [9]. As illustrated in the figure, the simulations using the deuteron sub-library reproduce the experimental data better than the simulations based on other models and data, especially at the forward angles. We have confirmed that these results are mainly due to differences in the treatment of the breakup processes and the (d,n) transfer reactions.

3 Alpha-particle sublibrary

Trans-uranium (TRU) elements and light elements (C, O, N, F, etc.) often coexist in situations such as storage and transportation of irradiated nuclear fuel. α-rays emitted from the decay of TRU nuclides can produce neutrons by interaction with surrounding light nuclei. Therefore, data on α-particle-induced neutron production reactions on light elements are important for radiation shielding and criticality safety in back-end facilities. Under these circumstances, JENDL/AN-2005 [10] have been developed and released in 2006. In JENDL/AN-2005, data on neutron production cross sections and energy and angular distributions of outgoing neutrons were evaluated for 17 light nuclides from Li to Si up to incident α-particle energy of 15 MeV. The upper energy limit of 15 MeV was set as a sufficiently large value for the decay α-ray energy from TRU nuclides.

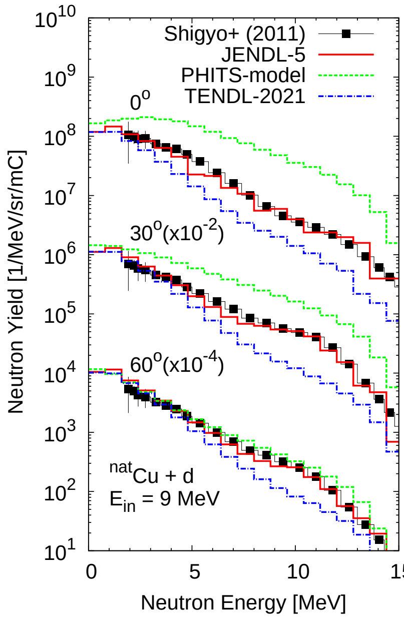

Figure 2. Same as Fig. 1 but for a thick natural copper target bombarded by a 9-MeV deuteron.

JENDL/AN-2005 was released more than 15 years ago, but even today there are few evaluated (α,n) reaction data on light nuclides. Fig. 3 shows the (α,xn) reaction cross sections on ^{18}O. The solid and dashed lines represent the data of JENDL/AN-2005 and TENDL-2021 [4], respectively. Experimental data are taken from Refs. [11, 12], and the ones by Bair et al. [12] are multiplied by 1.35. The necessity of the re-normalization was pointed out by Bair et al. themselves after the publication of the experimental data [13]. In the evaluation of JENDL/AN-2005, this information was taken into account. As shown in Fig. 3, the data of JENDL/AN-2005 reproduce the experimental ones well including resonance structures especially important for light nuclides. Also for the other nuclides, the (α,xn) reaction cross sections of JENDL/AN-2005 are in good agreement with experimental data.

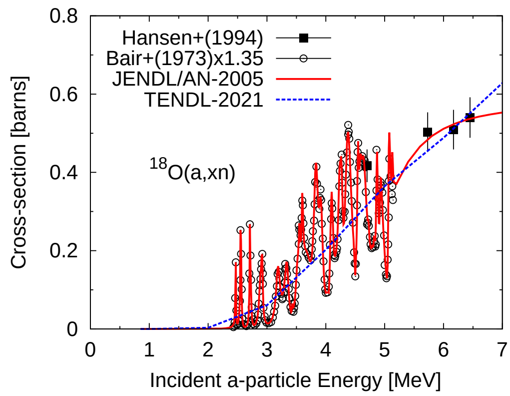

Figure 3. Experimental and evaluated (α,xn) reaction cross sections on ^{18}O.

However, in terms of energy distribution of neutrons produced from a thick target bombarded by -particles, it has been reported that large discrepancies are seen between experimental data and simulations based on JENDL/AN-2005 [14]. This suggest that the outgoing neutron energy distribution should be improved. Another issue is that JENDL/AN-2005 contains only data related to neutron emission. This means that the library cannot contribute to other applications such as simulation of -ray production. Simulation of -ray production is required for the quantitative analysis of actinides in the safeguards area. Moreover, due to the absence of data for elastic scattering and outgoing -particle spectra from the (, n) reaction, JENDL/AN-2005 cannot be processed with the NJOY code [15] properly. Therefore, ACE (A Compact ENDF) format le widely employed in the Monte Carlo transport codes such as PHITS [3] and MCNP [16] cannot be generate from JENDL/AN-2005.

To address the problems described above, the evaluation of -particle sub-library was made as follows. First, data up to 15 MeV were evaluated based on the calculations with the nuclear reaction code CCONE [17]. Then, only the cross sections of neutron production channels were replaced with those of JENDL/AN-2005. These procedures provide the following features: (1) neutron production cross sections of JENDL/AN-2005 are maintained, (2) energy and angular distributions of outgoing neutrons are evaluated with the CCONE code and improved from JENDL/AN-2005 (this is discussed in more detail in the next paragraph), (3) production of -rays from various reaction channels are included, and (4) ACE les can be generated by the processing with NJOY since elastic scattering and outgoing -particle spectra are included. In addition, we newly evaluated the data for ^{16}O, which are not included in JENDL/AN-2005 since neutron production channel is not open up to 15 MeV. ^{16}O has a large natural abundance (99.76%) and is expected to have a large impact especially on the estimation of -ray production.

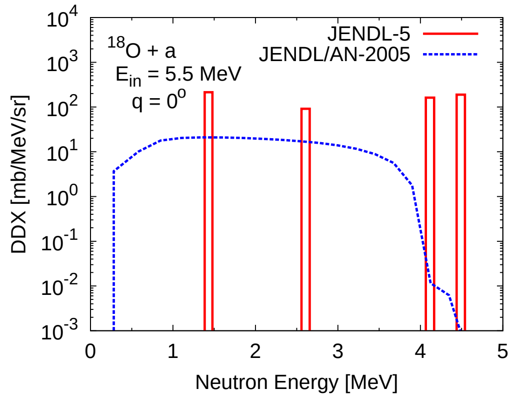

Figure 4. Comparison of double-di erential cross sections for the (, n) reactions on ^{18}O at 5.5 MeV. Emission angle is 0. The peaks of JENDL-5 are widened with a width of 0.1 MeV.

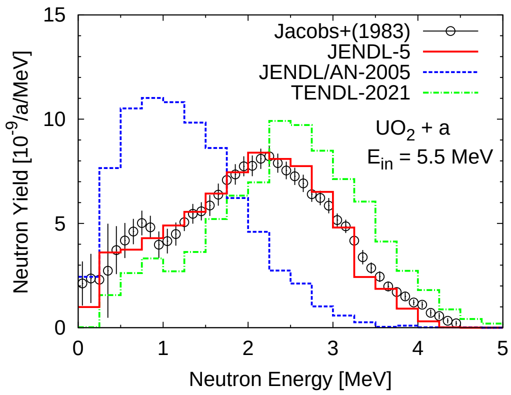

Figure 5. Experimental and calculated energy distribution of neutron yields from thick uranium dioxide (UO_2) target bombarded by a 5.5-MeV alpha-particle.

Figure 4 illustrates the double-di erential cross sections of (, n) reaction on ^{18}O at 5.5 MeV. The solid and dashed lines represent the data of the alpha-particle sub-library and JENDL/AN-2005, respectively. Note that the integral values for energy and angle are identical for both. As shown in the gure, the JENDL/AN-2005 evaluation gives continuous energy distributions for the (, n) reactions except for some nuclides. These energy distributions are based on the systematics by Kalbach and Mahn [18]. The Kalbach-Mahn systematics were developed mainly for the pre-equilibrium processes and the application to the compound processes involving the discrete states of residual nucleus is considered inappropriate. On the other hand, in the alpha-particle sub-library, the four peaks corresponding to the discrete states of residual nucleus ^{21}Ne are given.

For the validation of the alpha-particle sub-library regarding especially outgoing neutron spectrum, we perform transport simulation for the -particle-induced neutron yields from a thick target. Fig. 5 illustrates experimental and calculated neutron yields from thick uranium dioxide (UO_2) target, a compound of actinide and light element. Incident -particle energy is 5.5 MeV, which is a typical value for -ray energy from TRU nuclides. Experimental data are taken from Ref. [19]. The solid and dash-dotted lines represent the simulations with the PHITS code using the ACE les generated from the alpha-particle sublibrary and TENDL-2021, respectively. The dashed line is the simulation using the ACE les based on the JENDL/AN-2005. As already mentioned, JENDL/AN-2005 lacks data such as elastic scattering required for processing with NJOY. Therefore, these data are complemented by those of the alpha-particle sublibrary. The impact of these data on the transport simulation is expected to be limited. In the simulations based on the JENDL series, the ACE les for -particle of TENDL-2021 are employed for the uranium isotopes, although they have little e ect on the results.

As illustrated in Fig. 5, the simulation based on the alpha-particle sub-library reproduces the experimental data better than TENDL-2021 and much better than JENDL/AN-2005. For ^{16}O, no neutron emission channel is open up to 15 MeV as mentioned earlier. Considering the natural abundances of ^{17}O(0.04%) and ^{18}O(0.20%),

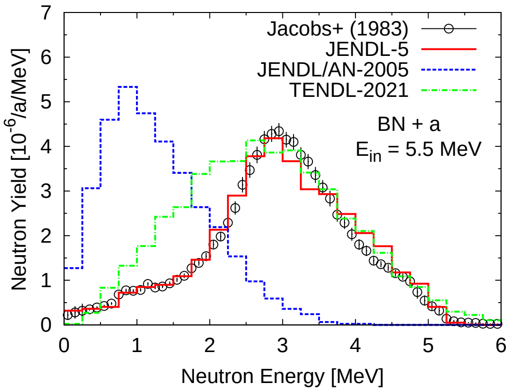

Figure 6. Same as Fig. 5 but for boron nitride (BN) target.

most of the neutron yields are the contribution from ^{18}O. These results demonstrate the validity of the outgoing neutron spectrum revised in the alpha-particle sub-library shown in Fig 4.

Similar validation result for boron nitride (BN) target is presented in Fig. 6. Experimental data are taken from Ref. [19]. Since the threshold energies of the -particle-induced neutron production from ^{14,15}N are greater than 5.5 MeV, the neutron yields are contributions from ^{10}B (natural abundance 19.9%) and ^{11}B (80.1%). Same as Fig. 5, the simulation based on the alpha-particle sub-library reproduces the experimental data better than those based on the other libraries.

4 Summary

We have outlined the evaluation and validation of the deuteron sub-library and the alpha-particle sub-library of JENDL-5.

The deuteron sub-library provides the data on light nuclides (^{6,7}Li, ^{9}Be, ^{12,13}C) and structural materials (^{27}Al, ^{63,65}Cu, ^{93}Nb) up to 200 MeV. The data for light nuclides were taken from JENDL/DEU-2020 with some modifications. The data for structural materials were newly evaluated employing the DEURACS code.

The alpha-particle sub-library provides the data for 18 light nuclides from Li to Si isotopes (^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12,13}C, ^{14,15}N, ^{16,17,18}O, ^{19}F, ^{23}Na, ^{27}Al, ^{28,29,30}Si) up to 15 MeV. The data were newly evaluated based on the calculations with the CCONE code, and then only the neutron production cross sections were replaced with the data of JENDL/AN-2005. By these procedures, the alpha-particle sub-library provides improved outgoing neutron spectrum data while keeping the evaluated neutron production cross section of JENDL/AN-2005. Furthermore, the completeness as a general-purpose particle library is enhanced by including data such as -ray and secondary particle production and elastic scattering.

For both sub-libraries, validation by particle transport simulation with the PHITS code was performed. The validation demonstrated that the simulations based on the sub-libraries of JENDL-5 were in good agreement with experimental data. These two sub-libraries are expected to contribute significantly to applications in a variety of fields.

Acknowledgment

The evaluation of the deuteron sub-library was partially supported by JSPS KAKENHI Grant Number 19K15483.

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