# Benchmark Calculation of d-Li Thick Target Neutron Yield by JENDL/DEU-2020 for IFMIF and Similar Facilities

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An accelerator-based neutron source using d-Li reactions is one of the most promising neutron sources for fusion material irradiation facilities such as IFMIF, where 40 MeV deuterons bombard a liquid lithium target. The neutron yield estimation including angular neutron spectra is one of the most important issues in the design of such irradiation facilities. Recently, JAEA released deuteron nuclear data of JENDL/DEU-2020 in ACE format file for Monte Carlo codes such as MCNP, and in Frag-Data format for the PHITS code. We carry out the benchmark calculations of d-Li neutron yield by using PHITS with Frag-Data, MCNP with JENDL/DEU-2020, and MCNP/PHITS with built-in nuclear reaction models. Those calculation results are compared with experimental data. It is confirmed that PHITS with Frag Data and MCNP with JENDL/DEU-2020 reproduce well the experimental data. Those are useful for the neutron yield estimation and also the irradiation field characterization of IFMIF and similar facilities.

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## 1. Introduction

Degradation of fusion materials such as embrittlement is one of the most serious issues on fusion reactors. In the fusion reactors, the embrittlement might be enhanced by helium gas production in the materials by n-$\alpha$ reactions. For the irradiation test of fusion materials, especially blanket structural materials, the International Fusion Materials Irradiation Facility (IFMIF) [1, 2] is under design by international collaboration. IFMIF is an accelerator-based neutron source where a couple of deuteron beams with 40 MeV and 125 mA bombard a flowing liquid lithium target as shown in Fig. 1. Also, design works of Advanced Fusion Neutron Source (A-FNS) [3] and DEMO-Oriented Neutron Source (DONES) [4], which are a half-size IFMIF with a single deuteron beam of 40 MeV and 125 mA, are advanced in Japan and EU, respectively.

An evaluation of the source neutron characteristics is one of the most important issues in the neutronics design of IFMIF and similar facilities. The neutron production process in the d-Li target is very complicated. Major neutron production reactions of d-Li are as follows;

$$\mathrm{d} + {}^{7}\mathrm{Li} \longrightarrow \mathrm{n} + {}^{8}\mathrm{Be} \qquad Q = 15.03\,\mathrm{MeV}, \tag{1}$$

$$\mathrm{d} + {}^{7}\mathrm{Li} \longrightarrow \mathrm{n} + {}^{8}\mathrm{Be}^{1} \qquad Q = 11.99\,\mathrm{MeV}, \tag{2}$$

$$\mathrm{d} + {}^{7}\mathrm{Li} \longrightarrow \mathrm{n} + 2\alpha \qquad Q = 15.12\,\mathrm{MeV}, \tag{3}$$

$$\mathrm{d} + {}^{6}\mathrm{Li} \longrightarrow \mathrm{n} + {}^{7}\mathrm{Be} \qquad Q = 3.38\,\mathrm{MeV}, \tag{4}$$

$$\mathrm{d} + \mathrm{Li} \longrightarrow \mathrm{n} + \mathrm{p} + \mathrm{Li} \qquad Q = -2.22\,\mathrm{MeV}, \tag{5}$$

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Because reactions of (1), (2), and (4) are two-body reactions, the energy of the emitted neutron is determined by kinematics. For the incident deuteron energy ($E_d$) of 40 MeV, the emitted neutron energy is 54.7 MeV, 51.6 MeV, and 42.5 MeV at 0 degrees for reactions (1), (2), and (4), respectively. Neutrons from reactions (3) and (5) have continuum energy spectra. In the case of the thick lithium target, the deuteron energy decreases from 40 MeV

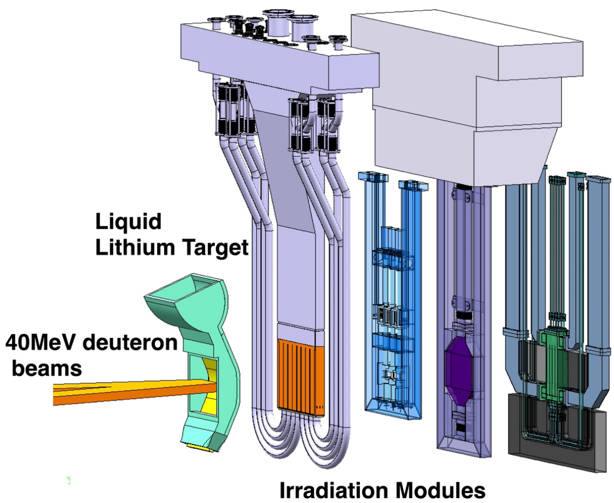


Fig. 1 Conceptual schematic view of the flowing liquid lithium target and the irradiation modules of IFMIF [1].



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to 0 in the target. Therefore, the emitted neutron has a wide continuum spectrum up to approximately 55 MeV. For the incident deuteron energy of 10 - 40 MeV, several nuclear reaction processes, compound nucleus formation, pre-equilibrium process, and direct reaction process, are mixed. Therefore, nuclear reaction simulation codes, such as MCNP (Monte Carlo N-Particle code) [5] and PHITS (Particle and Heavy-Ion Transport code System) [6] with generic nuclear reaction model could not predict the neutron yield, including angular neutron spectra, from d-Li reaction with sufficient accuracy.

The McDeLicious Monte Carlo code [7] has been developed by the Karlsruhe Institute of Technology group, which is concentrated on the prediction of d-Li neutron yield and used in the IFMIF design work. However, McDeLicious is not an open code. Therefore, more generic nuclear reaction simulation codes are desired for the d-Li neutron yield prediction. MCNP and PHITS calculate nuclear reactions with internal nuclear reaction model or nuclear cross-section library. If a nuclear cross-section library of d-Li reactions with sufficient accuracy is available, we can calculate the d-Li neutron yield with higher accuracy than built-in nuclear reaction models.

Recently, deuteron induced reaction library of JENDL/DEU-2020 [8] is released by the Japan Atomic Energy Agency (JAEA). We carried out the benchmark calculations of the d-Li neutron yield by using MCNP and PHITS with JENDL/DEU-2020, and also MCNP/PHITS with built-in nuclear reaction models. Those calculation results are compared with experimental data.

## 2. Calculation Tools

JENDL/DEU-2020 is released in three forms; ENDF format files [9], ACE (A Compact ENDF) format files [10], and Frag-Data [11]. The ENDF format is the most popular format to describe the nuclear reaction data. The ACE format file is proceeded by the NJOY code [12] from the ENDF format files for Monte Carlo codes. The Frag-Data is an external data file of the double differential cross-section table for PHITS.

MCNP is one of the most popular Monte Carlo codes in the world for neutron and other particles including photons. ITER adopts MCNP as a standard code for the shielding design. MCNP5 or earlier is mainly aiming at the transport calculation of neutrons lower than 20 MeV, photons, and electrons, using ACE files. MCNPX [13] is mainly aiming at the transport of many particles in the high-energy region, where particles reactions are calculated by built-in nuclear reaction models. ACE files are also available in MCNPX. MCNP6 merged previous MCNP and MCNPX. After that, MCNP can use not only ACE files but also built-in nuclear reaction models.

PHITS calculates many kinds of particles by ACE files, nuclear reaction models, and quantum molecular dynamics depending on the energy region. For the calculation using ACE files, PHITS is using MCNP4C. Present PHITS (version 3.24) carries out particle transport calculations by using ACE files only for neutrons, photons, electrons, and protons. PHITS could not use ACE files of deuteron-induced reactions. PHITS can use JENDL/DEU-2020 only by the Frag-Data. MCNP6.2, which is the latest version, can treat deuteron-induced reactions by ACE files. Therefore, we calculate the d-Li neutron yield by MCNP6.2 with ACE files and by PHITS with the Frag-Data. To compare those results, MCNP and PHITS calculations with embedded nuclear reaction models are carried out. In the MCNP calculations with a built-in reaction model, the ISABEL [14] intra-nuclear cascade model is employed. In the PHITS calculation, an Intra-Nuclear Cascade of Liége (INCL) model [15] and a combinationg of a INCL model and a Distorted Wave Born Approximation (DWBA) [16] are used, where the formula proposed by Minomo, Washiyama, and Ogata [17] (MWO formula) is adopted for the total cross-section of deuteron-induced reactions. For the validation confirmation, several experimental data from literature and EXFOR [18] database, and McDeLious calculation results [19] are referred to. Finally, we carried out five kinds of calculations; MCNP with JENDL/DEU-2020 ACE files, MCNP with the ISABE model, PHITS with Frag-Data based on JENDL/DEU-2020, PHITS with the INCL model, and PHITS with the INCL and DWBA models. In this study, MCNP version 6.2 and PHITS version 3.24 are used.

In those calculations, a pencil deuteron beam bombards a natural lithium target with 20 mm in diameter and 25 mm in thickness. The 45 MeV deuteron beam fully stops in the target, because the range of 45 MeV deuteron is approximately 24 mm. Cell tallies of cylindrical geometry with 170 mm in diameter and 10 mm in thickness are located on the circle 1 m far from the target at 0 degrees to 180 degrees with 10 degrees pitch against the incident beam direction. In experiments for the benchmark [18–21], similar size of the lithium target was used. Many of those experiments used the Time-of-Flight methods with typical fight path of 10 m. The distance between the target and tallies (detectors) in calculations is much shorter than that of experiment to increase statistics.

## 3. Results

### 3.1 Forward neutron yields

In the application to IFMIF and similar facilities, a neutron yield in the forward direction is more important than the total neutron yield. Figure 2 shows calculated forward neutron yields as a function of the incident deuteron energy compared with experimental data [18–21] and the McDeLious calculation results [19]. In the calculated forward neutron yields, the curve shapes of the incident energy dependence are similar except PHITS with the INCL and DWBA models (PHITS with INCL + DWBA). Absolute values of MCNP with JENDL/DEU-2020, PHITS

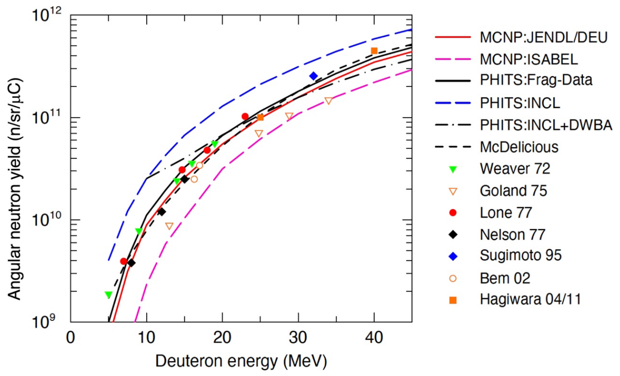


Fig. 2 Calculated forward neutron yields of the d-Li thick target as a function of the incident deuteron energy compared with experimental data and the McDeLious calculation results.

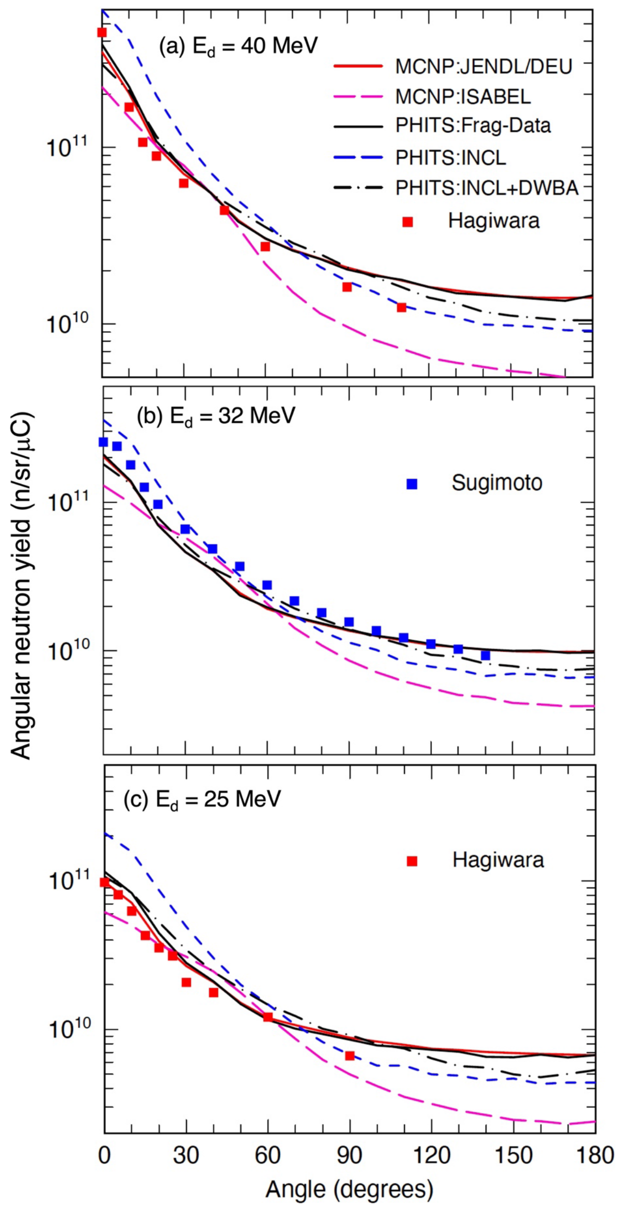


Fig. 3 Calculated and measured angular neutron yields of the d-Li thick target as a function of neutron emission angle for incident deuteron energy of (a) 40, (b) 32, and (c) 25 MeV.

with Frag-Data, and McDeLicious are in good agreement with experimental neutron yields. The reason for the small difference between MCNP with JENDL/DEU-2020 and PHITS with Frag-Data is considered due to the difference of the conversion process of the Frag-Data and the ACE fail, and interpolation method for Frag-Data and ACE files in PHITS. PHITS with INCL overestimates forward neutron yields approximately factor 2 compared with the experimental data. On the other hand, MCNP with ISABEL agrees with Goland's data, however, underestimates approximately 50% compared with the other experimental data. PHITS with INCL + DWBA is in good agreement with experimental data in the incident energy range of 20 - 35 MeV.

### 3.2 Angular neutron yields

Angular neutron yields of the d-Li thick target including double-differential neutron yield (angular dependent neutron energy distribution) have been measured by Hagiwara [20] at 40 MeV and 25 MeV, Sugimoto [21] at 32 MeV, and Bém [19] at 17 MeV. Especially, Hagiwara and Sugimoto measured the angular neutron yield at many emission angles at the Cyclotron RI Center of Tohoku University and Tandem Van de Graaff accelerator of JAEA, respectively. Therefore, we compared our calculation results with the experimental data by Hagiwara and Sugimoto.

Figure 3 shows the calculated and measured angular neutron yields of the d-Li thick target as a function of neutron emission angle for incident deuteron energy ($E_d$) of 40, 32, and 25 MeV. In this paper, the neutron emission angle is in the laboratory system. The statistical error of calculations is smaller than 1%. MCNP with JENDL/DEU and PHITS with Frag-Data are almost identical. Both are in good agreement with Hagiwara's data for the $E_d$ of 40 and 25 MeV, especially at the forward directions. Those are slightly underestimation compared with Sugimoto's data in the forward directions at $E_d$ of 32 MeV. The angular dependence of MCNP with ISABEL and PHITS with INCL is more forward directional compared with the experimental data and other calculation results. It is interesting that PHITS with INCL + DWBA is in rather good agreement with the experimental data.

### 3.3 Double differential neutron yields

In the fusion material irradiation experiment, not only neutron flux but also neutron energy spectrum is important. It is well known that IFMIF and similar facilities have the fusion relevant neutron spectrum, almost 14 MeV, however, has a higher energy tail up to 60 MeV. The higher energy tail than 20 MeV causes many transmutation reactions, which do not occur under the fusion reactor environ-

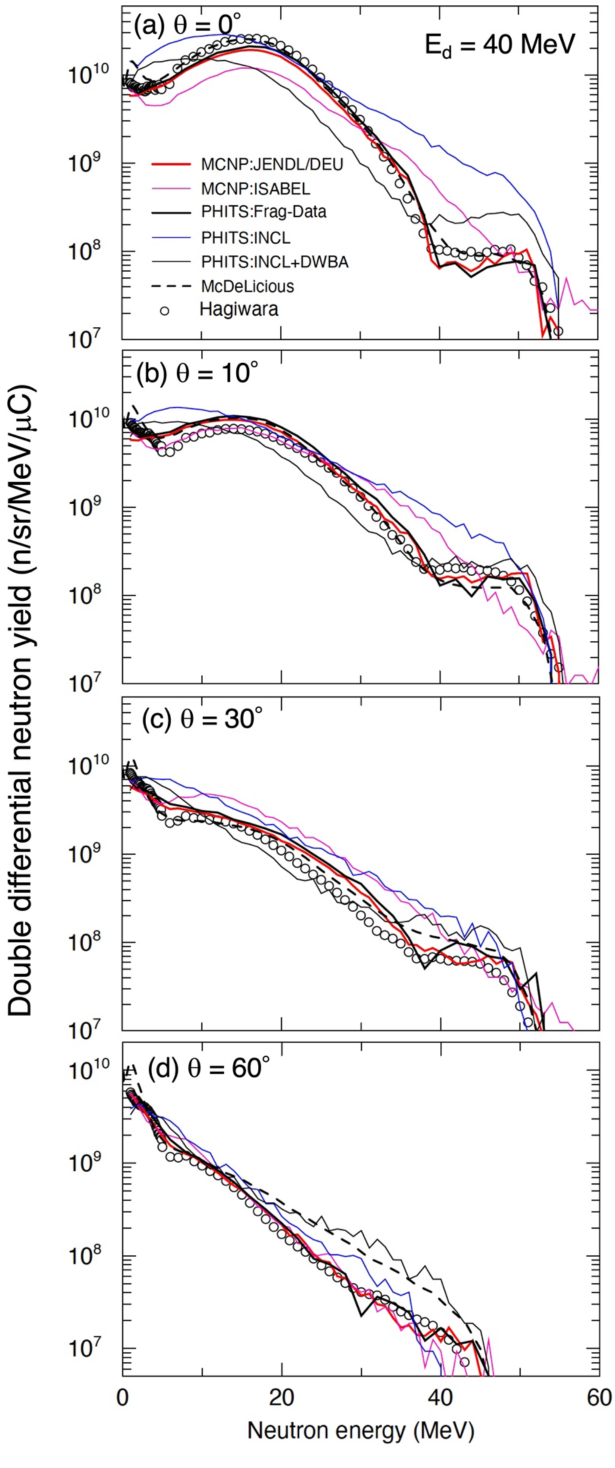


Fig. 4 Calculated and measured double-differential neutron yields of the d-Li thick target at (a) 0, (b) 10, (c) 30, and (d) 60 degrees for incident deuteron energy of 40 MeV.

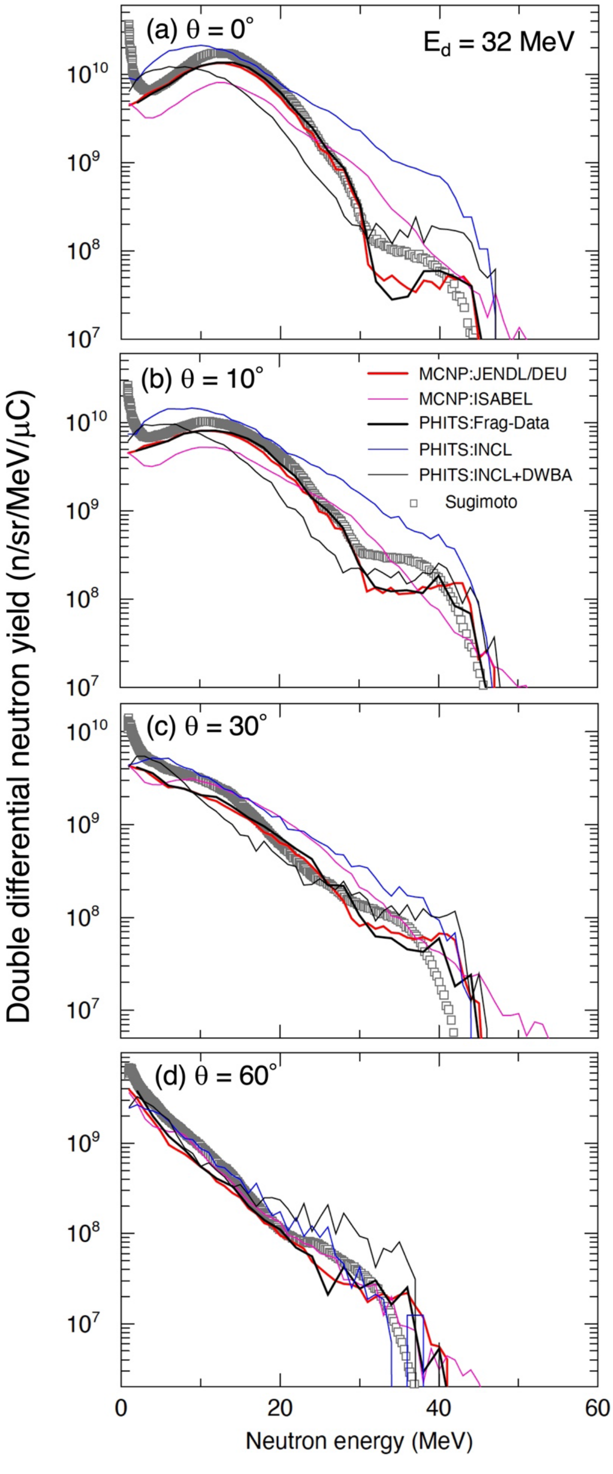


Fig. 5 Calculated and measured double-differential neutron yields of the d-Li thick target at (a) 0, (b) 10, (c) 30, and (d) 60 degrees for incident deuteron energy of 32 MeV.

ment. Therefore, the evaluation of the neutron spectrum not only around 14 MeV but also a higher energy tail is necessary.

Figures 4 - 6 show the calculated and measured double-differential neutron yields of the d-Li thick target at 0, 10, 30, and 60 degrees for $E_d$ of 40, 32, and 25 MeV. The double-differential neutron yields for $E_d$ of 40 and 25 MeV were measured by Also, double-differential neutron yields calculated with McDeLicious, which is used in the IFMIF design, are plotted for $E_d$ of 40, and 25 MeV. For $E_d$ of 40 and 25 MeV, McDeLicious reproduces experimental data of Hagiwara remarkably, which is considered that McDeLicious has been adjusted to the ex-

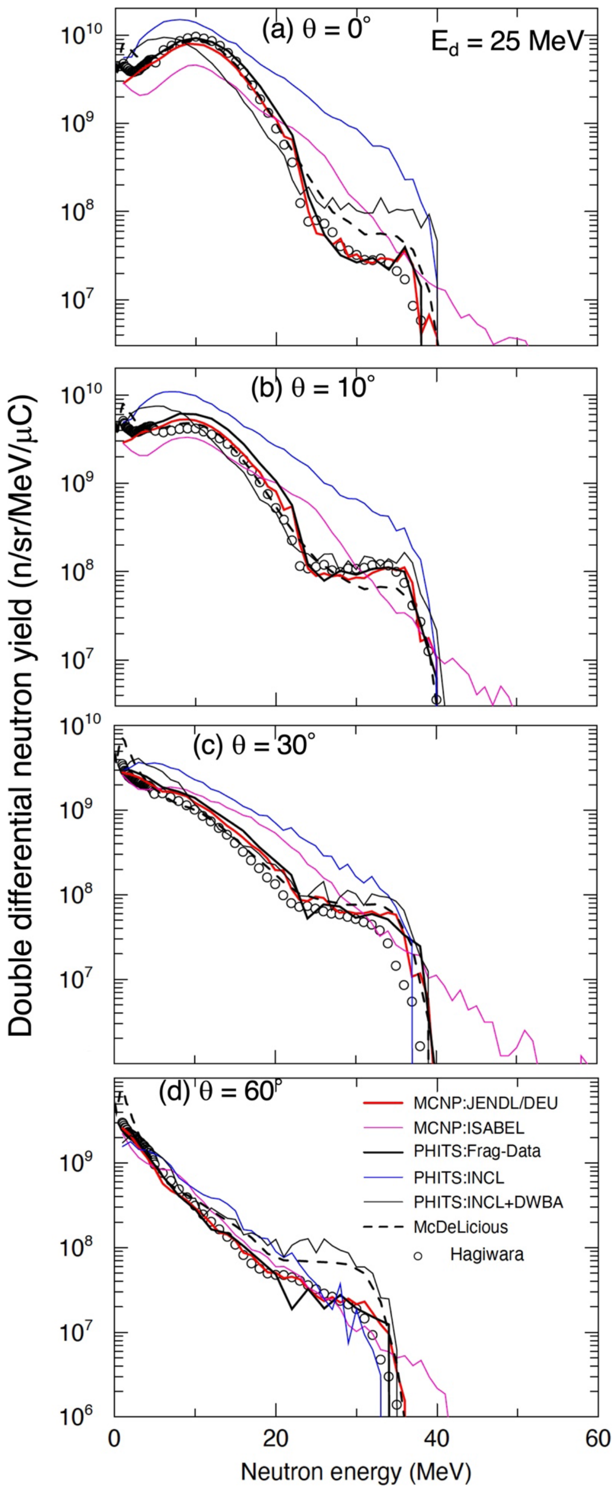


Fig. 6 Calculated and measured double-differential neutron yields of the d-Li thick target at (a) 0, (b) 10, (c) 30, and (d) 60 degrees for incident deuteron energy of 25 MeV.

perimental data for the IFMIF design. Also, MCNP with JENDL/DEU and PHITS with Frag-Data are in good agreement with the experimental data of Hagiwara and Sugimoto. A significant rise of the neutron flux at energies close to 0 MeV is seen in Fig. 5, but not seen in Figs. 4 and 6. The experimental setup of Sugimoto's experiment is not clear from the literature. It seems that the detectors are well shielded in Hagiwara's experiment. The possible reason for the significant rise close to 0 MeV is gamma-ray or electrical noise contamination in low-energy regions. The main peak in PHITS with INCL and PHITS with INCL + DWBA is shifted to lower energy approximately 5 - 10 MeV from the main peak of the experimental data. The main peak energy is very important as a fusion-relevant neutron source. In PHITS with INCL + DWBA, a higher energy peak/shoulder around 50 MeV is seen, however, the intensity is overestimated compared with the experimental data. The main peak energy of MCNP with ISABEL is almost the same as the experimental data, however, the intensity is lower than the experimental data.

## 4. Conclusion

We carry out the benchmark calculations of d-Li neutron yield including angular dependent neutron spectra by using PHITS with Frag Data based on JENDL/DEU-2020, MCNP with ACE format files of JENDL/DEU-2020, and MCNP/PHITS with built-in nuclear reaction models. It is found that PHITS with Frag-Data and MCNP with JENDL/DEU-2020 reproduce well the experimental data as well as McDeLocious. MCNP/PHITS with built-in nuclear reaction models do not have sufficient accuracy for the IFMIF design. PHITS with INCL + DWBA is available in limited applications such as neutron yield estimation except for angular neutron spectra.

By the information from the PHITS office, PHITS will be able to use ACE files of deuteron induced reactions such as JENDL/DEU-2020 in the next release of PHITS. FENDL 3.2, which is the nuclear data library compiled by IAEA for the fusion application, adopted JENDL/DEU-2020 as a part of FENLD-3.2 deuteron reaction cross-sections. Finally, we conclude that widely-used Monte Carlo codes such as PHITS and MCNP by using JENDL/DEU-2020 including JENDL/DEU-2020-based Frag-Data are useful tools for the neutronics design of IFMIF and similar facilities.

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