Benchmarking GEANT4 and PHITS for 14.8-MeV neutron transport in polyethylene and graphite materials

X. Zhang[a,b,c], Z. Chen[a,b,c,*], R. Han[a,b,c], G. Tian[a,c], B. Liu[a,b,c], F. Shi[a,c], H. Sun[a,b,c], R. Wada[d]

[a] *Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, 730000, China*
[b] *School of Nuclear Science and Technology, University of Chinese Academy of Science, Beijing 100049, China*
[c] *Advanced Energy Science and Technology Guangdong Laboratory, Huizhou, 516000, China*
[d] *Cyclotron Institute, Texas A&M University,College Station, Texas 77843, USA*

Abstract

The feasibility of GEANT4 and PHITS with ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0 evaluated nuclear data libraries in 14.8-MeV neutron transport simulation are verified by comparing with the MCNP calculations and the experimental data. The measured data are from neutron integral experiments including graphite and polyethylene samples. For 6 cm-thick polyethylene and 20 cm-thick graphite samples, the results from GEANT4 and PHITS with three evaluated nuclear data libraries agree well with the MCNP calculations. For a 2 cm-thick graphite sample, the simulated results from GEANT4 and PHITS agree with the MCNP calculations, and they all underestimate the experiment data in below 3 MeV and overestimate them in the energy range of 5-7 MeV. The difference between the simulation results and the experimental data depends on the evaluated nuclear data libraries. In overall, GEANT4 and PHITS are performing reasonable jobs for 14.8-MeV neutron transport simulations.

Keywords: neutron transport, GEANT4, PHITS

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1. Introduction

Monte Carlo simulation codes have been considered as an essential tool for solving the particle transport problems in space applications, nuclear reactor designing and its optimization, accelerator shielding and radiation protections. Using random sampling and probability techniques, these codes show the capability to estimate neutron transport characteristics, such as the neutron flux, energy spectrum and spatial distribution. There are several widely used Monte Carlo simulation codes, such as MCNP[1], GEANT4[2], and PHITS[3] [4]. MCNP developed in the Los Alamos National Laboratory can be used to calculate complex

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[*] Corresponding author
Email address: `zqchen@impcas.ac.cn` (Z. Chen)

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systems and solve three-dimensional particle transport problems accurately. GEANT4 is an open-source software toolkit for the simulation of particles transport in matter. It was originally used to simulate high-energy particle detection systems and has been extended for the neutron transport simulations below 20 MeV with the neutron transport physics models and the evaluated nuclear data libraries. PHITS is a general purpose code to simulate particles and heavy ions transport in materials with energy up to 1 TeV (per nucleon for ion) by utilizing different nuclear reaction models and evaluated nuclear data libraries. The benchmark and validation of these codes are very important in practical applications. Based on a large amount of experimental validations, the MCNP code has been considered as a standard tool for neutron transport simulations below 20 MeV. However, only few investigations about the neutron transport below 20 MeV in GEANT4 have been reported [5–10], and even fewer for PHITS. Recently Nunnenmann et al. [9] reported the validity of GEANT4 for the experimental benchmark on iron shells. They concluded that GEANT4 is suitable for the fusion applications, but there are still some discrepancies, compared to the experimental data. For the better verification and validation analyses of simulation codes, more neutron integral experiments are needed. Series of such experiments, including polyethylene and graphite samples, have been carried out using the neutron benchmark experimental facility at China Institute of Atomic Energy (CIAE) [11]. In our previous works [12, 13], the benchmark of the evaluated nuclear data libraries were performed with MCNP by comparing with the experimental leakage neutron spectra. In this work, polyethylene and graphite, which are very important for the nuclear engineering applications, are selected and their leakage neutron spectra are compared with GEANT4 and PHITS simulations with ENDF/B-VIII.0 [14], JEFF-3.3 [15] and JENDL-4.0 [16] libraries, aiming at verifying the feasibility and reliability of GEANT4 and PHITS for simulating 14.8-MeV neutron transport.

2. Neutron Integral Experiments

The experiments were conducted using the neutron benchmark experimental facility at CIAE. A layout of the experiment setup is presented in Fig. 1. Neutrons with energy about 14.8 MeV were produced through the $\mathrm{T}(d,n)^4\mathrm{He}$ reactions. An Au-Si surface barrier semiconductor detector was used to count the associated alpha particles to monitor the intensity of the source neutrons. A beam pick-up detector (Faraday cup) was placed near the T-Ti target. One polyethylene cylinder sample (ϕ = 13 cm, length = 6 cm, density = 0.95 g/cm^3) and two graphite cylinder samples (ϕ = 13 cm, length = 2 cm and 20 cm, density = 1.8 g/cm^3) were used in the experiments. The sample was placed at 33 cm from the T-Ti target. The leakage neutron spectra were measured at 60° by a BC501A neutron detector located at about 8 m from the sample behind a concrete wall. A copper shadow bar with length of 90 cm was used to prevent the source neutrons injecting into the BC501A detector directly. A collimator system consisted of iron, polyethylene and lead was used. The leakage neutron time-of-flight (TOF) spectra were measured, and then converted into energy spectra. More detailed experimental information can be found in Luo et al. [12].

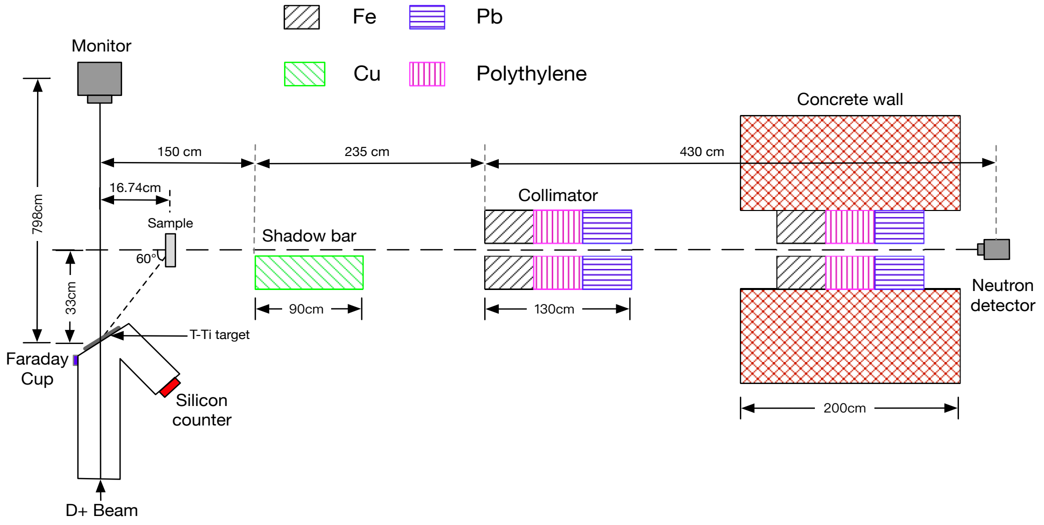

Figure 1: A schematic drawing of the neutron integral experiment setup.

3. The simulation toolkits

GEANT4 toolkit is a well-established Monte Carlo simulation code, written in C++. Its modifiability and extensibility make it widely used in nuclear medicine, space physics, reactor physics, accelerator design, radiation protection etc. GEANT4 provides different physics modules and the usage of the evaluated nuclear data libraries to simulate neutron transport in materials. The neutron interaction with matter in GEANT4 is divided into four separate processes including elastic scattering, inelastic scattering, radiative capture, and fission [17]. The recommended PhysicsList for neutrons with energy below 20 MeV is the "G4NeutronHP package" [18], which allows using the evaluated nuclear data libraries in the G4NDL format. This PhysicsList can use either tabulated differential cross-sections or a series of Legendre polynomials to sample the energy and angular distribution based on the evaluated data libraries. In recent years, Mendoza et al. [19] convert the ENDF-6 formatted libraries into a GEANT4's accepted G4NDL format. In this work, ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0 libraries and GEANT4-v.10.05.p01 are used for the calculations.

PHITS is a Monte Carlo particle transport simulation code developed under collaboration between JAEA, RIST, KEK and several other institutes, and it is written in Fortran [20]. Using several nuclear reaction models and the evaluated nuclear data libraries, it can deal with particle transport over wide energy ranges and has been applied in a wide field. For neutron-induced reactions below 20 MeV, PHITS firstly samples reactions from reaction-channel (elastic and inelastic scattering, etc.) cross sections and then determines the energy, momentum and scattering angle of the scattered neutrons according to the cross sections given in the evaluated data libraries. The evaluated data libraries format in PHITS are written in the ACE format, which is identical to the data library format in MCNP. PHITS v3.20 was used in the present work.

The MCNP5 version 1.60 was used for this study. The energy distributions of the neutrons emitted from the $T(d,n)^4He$ source in different angles have been simulated using TARGET code[21]. The calculated results are given in Fig.2. The energy-angle distribution of source neutrons was generated by in the MCNP and PHITS input file. In GEANT4, the energy-angle distribution of source neutron was hardcored into the GeneralParticleSource input file. For speeding up calculations, the "simplified simulation" was used in MCNP. The transport region of leakage nuetrons in the ideal collimator system was limited by a cylindrical tube with the radius same as the experimental collimator system (Fig. 3). The calculation time of the "detailed simulation" (with collimators) is about five times of the "simplified simulation", and the difference between their results is less than 2% from [11]. In GEANT4 and PHITS modeling configuration, a sample setup contained target, sample and detector was used (Fig. 4). In order to prevent the source neutrons from entering the detector directly, source neutrons entering the outer region of the sample were subtracted from the angular distribution. In MCNP, a point detector with F5 tally card was used to record leakage neutron. In GEANT4, a standard sensitive detector of actual size was chosen to record leakage neutron spectra. In PHITS, "T-track" tally card, a similar recording method with the sensitive detector in GEANT4, was used to record neutron spectra in the detector cell.

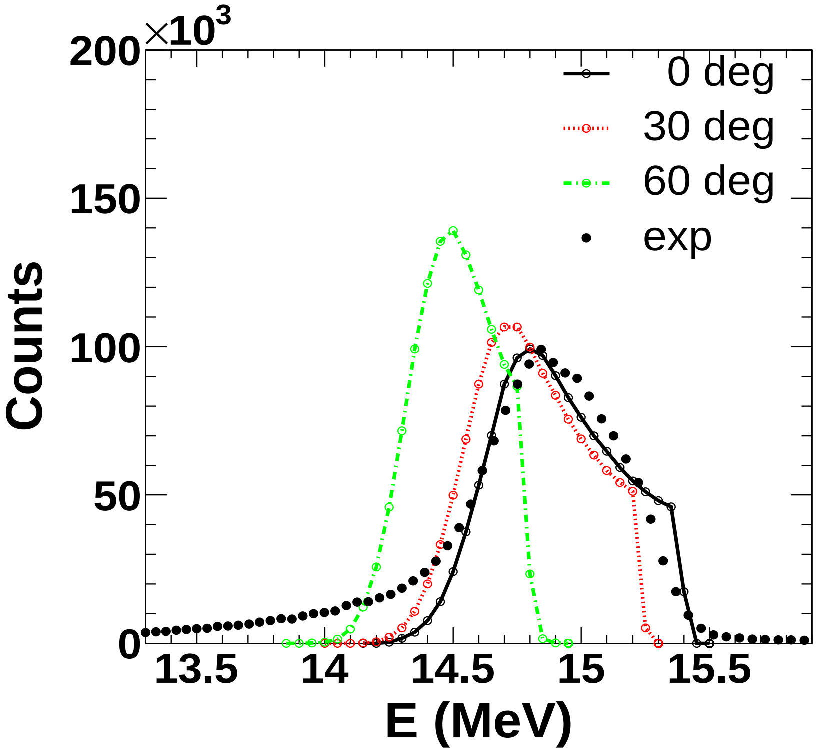

Figure 2: Energy spectrum of the source neutrons in different angles predicted by TARGET code

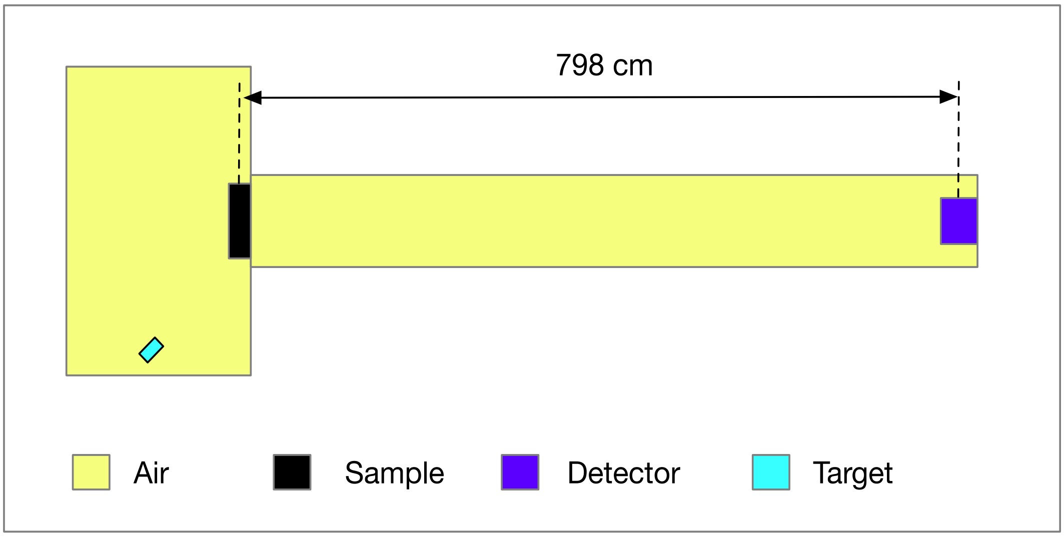

Figure 3: The models in MCNP simulations

4. Results and discussion

4.1. 6 cm-thick polyethylene sample

The leakage neutron spectrum of experiments and simulations, and calculation-to-experiment (C/E) ratios for the 6 cm-thick polyethylene sample are shown in Fig. 5. The simulations are performed by GEANT4, PHITS and MCNP with ENDF-VIII.0, JEFF-3.3 and JENDL-4.0 libraries. The C/E ratios are performed the yields integrated over the three major peaks in the neutron energy (E_n) range of 1.0-7.0, 7.0-11.0, 11.0-15.0 MeV, respectively. The results show that GEANT4 and PHITS calculations agree well with MCNP ones. In the energy range below 11 MeV, all simulated results and the experimental data are agree within less than a few tens%. In the energy range of 11-15 MeV, these simulation codes with ENDF/B-VIII.0 and JEFF-3.3 libraries overestimate the experimental data by $\sim 50\%$, while the results from JENDL-4.0 library show a slightly better agreement ($\sim 20\%$) with the experimental data.

4.2. 2 cm-thick graphite sample

The leakage neutron spectrum of experiments and simulations, and calculation-to-experiment (C/E) ratios for a 2 cm-thick graphite sample are shown in Fig. 6. The C/E comparisons are made around five different energies, ranging from 1-3, 3-5, 5-7, 7-11 and 11-15 MeV. In general, the agreements among GEANT4, PHITS and MCNP calculations becomes slightly worse than those in the previous case in the whole energy range. In the energy range of 1-3 MeV, the calculated values from simulation codes with ENDF/B-VIII.0 and JEFF-3.3 libraries underestimate the experimental data by $\sim$ 60% for GEANT4 and PHITS, whereas those from JENDL-4.0 library show a good agreement with experimental data for all simulation codes. In the energy range of 5-7 MeV, GEANT4, PHITS and MCNP with three data libraries all show a small peak and overestimate the experimental data by $\sim 20\%$ to

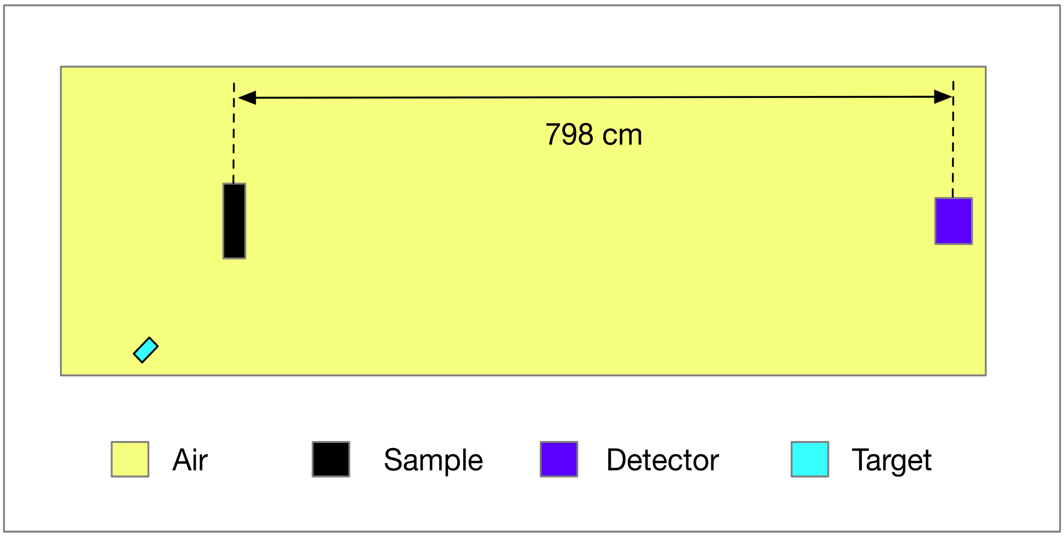

Figure 4: The models in GEANT4 and PHITS simulations

80%. According to previous works [12, 13, 22], it pointed out that this peak is caused from inelastic scattering of the second excited state of carbon and it has significant angular dependence and would disapear at large angle. For the thick graphite case in the next subsection, this peak is smeared out and disappears. This overestimate at 5-7 MeV energy range was mainly caused by the evaluated data. At the energy range between 7 to 11 MeV, all simulated results agree with the experimental data better than 20%, and in the energy above 11 MeV, all simulations with ENDF/B-VIII.0 and JEFF-3.3 overestimates the experimental values by $\sim$ 20%, but those with JENDL-4.0 reproduce the experimental values within the error bars. Among these simulations, the simulations with JENDL-4.0 shows the minimum deviation and especially with PHITS, the results agree with the experimental data within the error bars in the entire energy range except for 5-7 MeV, where it shows $\sim$ 40%.

4.3. 20 cm-thick graphite sample

The results for a 20 cm-thick graphite sample are shown in Fig. 7. The C/E values are calculated in four energy ranges, 0-3, 3-7, 7-11, 11-15 MeV. All simulations agree well in each other within the error bars and the deviation from the experimental data also is $\sim$ 10% at most except for those with ENDF/B-VIII.0 and FEFF-3.3 in the energy lower than 3 MeV. The simulations with JENDL-4.0 agree with each other within the error bars in the entire energy range and the agreement with the experimental data are within a few 10%. GEANT4, PHITS and MCNP underestimate the valley around 10.5 MeV $< E_n <$ 12 MeV and the yields at $E_n >$ 15 MeV. This difference need further investigations.

5. Conclusion

In this work, GEANT4 and PHITS with ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0 nuclear data libraries are used to simulate the leakage neutron energy spectra of D-T neutrons bombarding polyethylene and graphite samples and the results are compared with

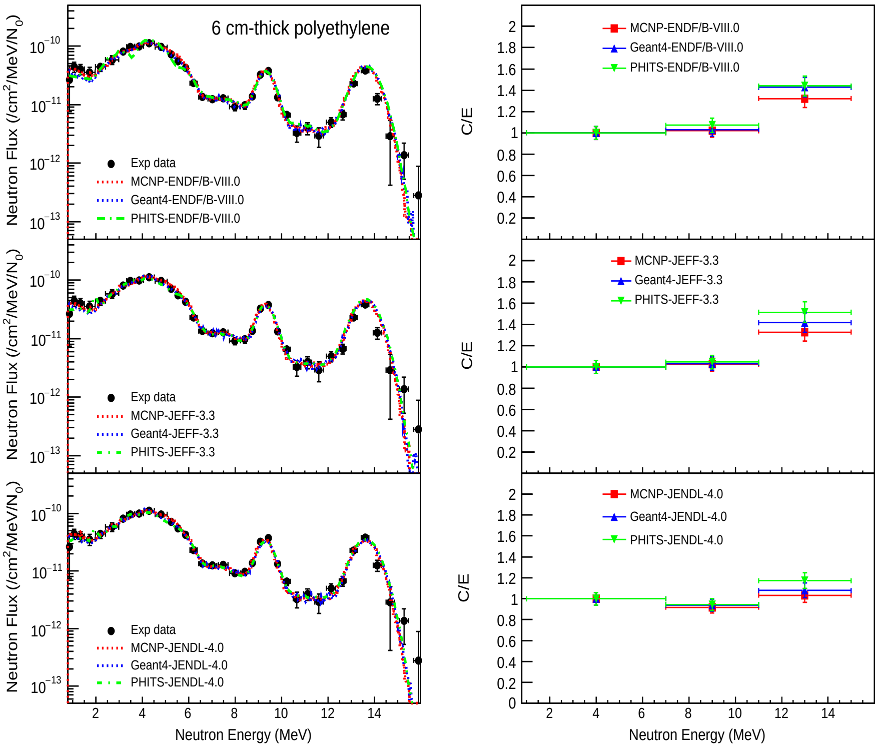

Figure 5: (Left) The leakage neutron spectra measured in the experiment and simulated by GEANT4, PHITS and MCNP codes for the 6 cm-thick polyethylene sample. (Right) The C/E ratios for simulation results over experimental data at given energy ranges.

those of MCNP and the experimental data. For 6 cm-thick polyethylene and 20 cm-thick graphite samples, the calculated results of GEANT4 and PHITS agree well with MCNP ones. The simulations with JENDL-4.0 show better agreement with the experimental data. For the 2 cm-thick graphite sample, the calculated results of GEANT4 and PHITS with ENDF/B-VIII.0 and JEFF-3.3 show largest deviation among the simulations and from the experimental data. The simulated results from GEANT4, PHITS and MCNP calculations all underestimate the experiment data in below 3 MeV and overestimate in the energy range of 5-7 MeV. On the other hand, three simulations with JENDL-4.0 agree well in each other and deviations from the experimental data are within the error bars in the entire energy range except 5-7 MeV. For thick sample, these simulation codes could get identical results for neutron transport calculation. Overall, it is reliable to use GEANT4 and PHITS to simulate the transport of 14.8-MeV neutron in polyethylene and graphite materials with ENDF/B-VIII.0, JEFF-3.3, and JENDL-4.0 evaluated data libraries. And further validations of GEANT4 and PHITS for more materials should be performed.

Acknowledgments

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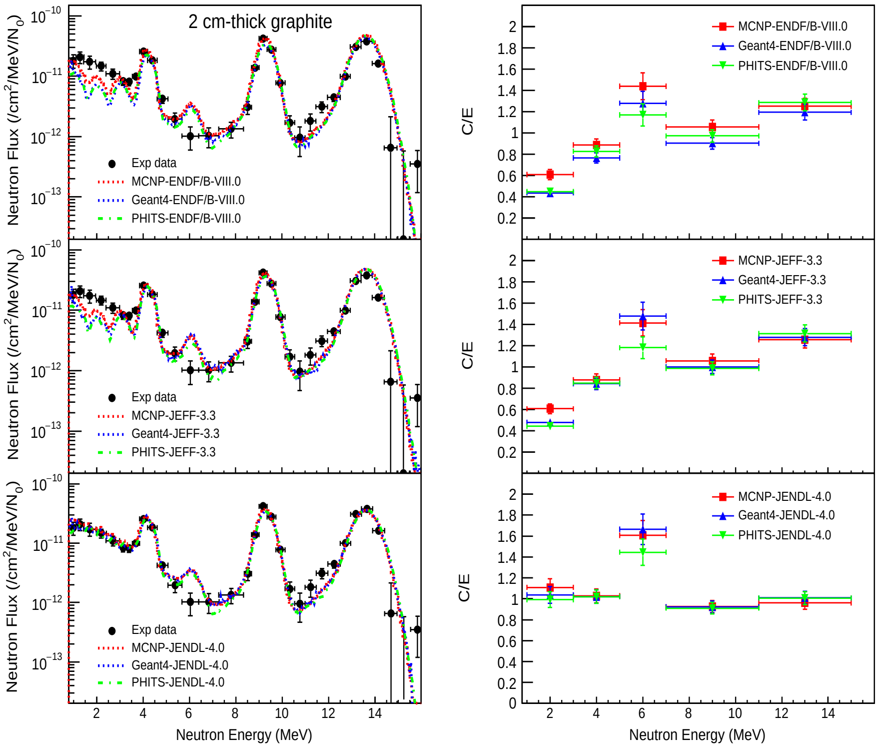

Figure 6: Similar plots as those in Fig.5, but for the 2 cm-thick graphite sample. The C/E is calculated in five different energy ranges as shown.

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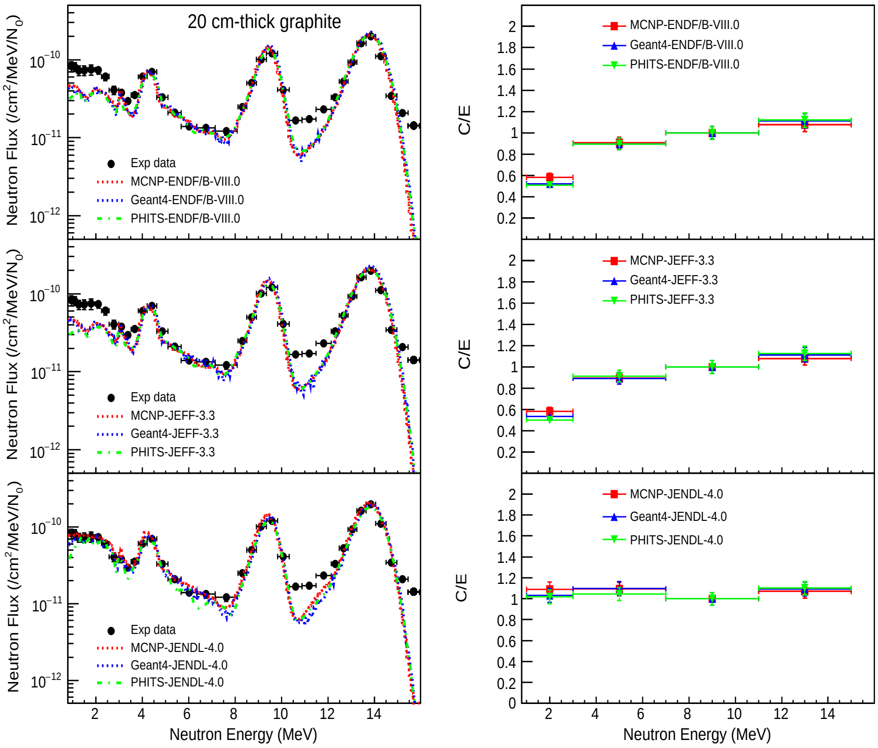

Figure 7: Similar plots as those in Fig.5, but for the 20 cm-thick graphite sample. C/E is made at four different energy ranges.

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