Nuclear Data Evaluation for JENDL High Energy File and Its Benchmark

Yukinobu Watanabe
Department of Advanced Energy Engineering Science, Kyushu University,
Kasuga, Fukuoka 816-8580, Japan
Corresponding email: watanabe@aees.kyushu-u.ac.jp

An overview is reported of nuclear data evaluation for the JENDL High Energy (JENDL-HE) file which contains neutron and proton cross sections for energies up to 3 GeV for the whole 132 nuclides. The JENDL-HE evaluations are performed on the basis of experimental data and theoretical model calculations. For the cross section calculations, a hybrid calculation code system is constructed using some available nuclear model codes and systematics-based codes. The evaluated cross sections are compared with available experimental data and the other evaluations. Some preliminary results of benchmark tests are also presented.

1. Introduction

In recent years, nuclear data for energies over 20 MeV are needed from the point of view of accelerator-related applications, such as accelerator-driven transmutation system, radiotherapy with particle beams, and estimation of radiation effects induced by cosmic rays in microelectronics, *etc*. These applications require charged-particle data, particularly proton data, as well as neutron data in macroscopic transport and activation calculations. Under these backgrounds, there are several activities on high-energy nuclear data evaluations in LANL, NRG Petten, FZK, IPPE, KAERI and so on. Some of the data libraries produced in these evaluations are currently available. Among them, the LA150 library[1] is widely used in macroscopic transport calculations, which treats the nuclear interaction of neutrons and protons having energies up to 150 MeV with materials. In such calculations, the Monte Carlo codes based on microscopic simulation approach such as the intra-nuclear cascade model are built-in to deal with the nuclear processes at energies above 150 MeV, instead of the nuclear data library. Because of saving the computation time, however, the nuclear data above 150 MeV are also required in macroscopic transport and activation calculations. Thus, the Japanese Nuclear Data Committee (JNDC) has launched the JENDL High-Energy file (JENDL-HE) project[2], in which the cross sections for neutron and proton induced reactions up to 3 GeV are included for the total 132 nuclides shown in **Table 1**.

In this paper, the current status of the JENDL-HE file is reported with an outline of a nuclear model calculation code system used in the evaluation and comparisons of the JENDL-HE evaluation with available experimental data and other evaluations. Preliminary results of some benchmark tests using the transport code MCNPX are also given.

Table 1. List of nuclides to be included in JENDL High Energy file

Released (66 nuclides)	^{1}H, ^{12,13}C, ^{14}N, ^{16}O, ^{24,25,26}Mg, ^{27}Al, ^{28,29,30}Si, ^{39,41}K, ^{40,42,43,44,46,48}Ca, ^{46,47,48,49,50}Ti, ^{51}V, ^{50,52,53,54}Cr, ^{55}Mn, ^{54,56,57,58}Fe, ^{59}Co, ^{58,60,61,62,64}Ni, ^{63,65}Cu, ^{64,66,67,68,70}Zn, ^{90,91,92,94,96}Zr, ^{93}Nb, ^{180,182,183,184,186}W, ^{196,198,199,200,201,202,204}Hg
In prepartion (66 nuclides)	^{2}H, ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{15}N, ^{18}O, ^{19}F, ^{23}Na, ^{35,37}Cl, ^{35,38,40}Ar, ^{69,71}Ga, ^{70,72,73,74,76}Ge, ^{75}As, ^{74,76,77,78,80,82}Se, ^{89}Y, ^{92,94,95,96,97,98,100}Mo, ^{113,115}In, ^{197}Au, ^{204,206,207,208}Pb, ^{209}Bi, ^{232}Th, ^{233,234,235,236,238}U, ^{237}Np, ^{238,239,240,241,242}Pu, ^{241,242,242m,243}Am, ^{243,244,245,246}Cm

2. Nuclear model calculation code system

In the present JENDL-HE evaluation, a model calculation code system combining some nuclear model codes is used to produce the high-energy cross section data. A schematic diagram of the code system is illustrated in **Fig.1**. It consists of two different parts in accordance with the incident energy. For energies below 150-250 MeV, the conventional codes used widely in the evaluations below 20 MeV are applied, and

Monte Carlo calculation codes based on the intra-nuclear cascade (INC) model or quantum molecular dynamics (QMD) are used mainly for those above 150-250 MeV.

The main code for energies below 150-250 MeV, GNASH[3], is based on statistical Hauser-Feshbach plus preequilibrium exciton models to predict nuclear reaction cross sections for particle and γ-ray emissions. A modified version of the code EXIFON[4] is used as an alternative code for N and O as well. The optical model is employed for predictions of the total, reaction, and elastic scattering cross sections. Optical model calculations are carried out using ECIS96[5] or OPTMAN[6]. The code OPTMAN is based on the coupled-channels method with the nuclear Hamiltonian parameters determined by the soft-rotator model, and is used only for C, Mg, and Si. Transmission coefficients provided by the optical model calculation are employed in the GNASH calculations of particle and γ-ray emission cross sections and isotope production cross sections. The cross sections for inelastic scattering to low-lying excited states are also calculated using ECIS96 or OPTMAN. For some cases, the code DWUCK4[7] based on DWBA is used for direct reaction calculations for discrete state transitions including deuteron pick-up and charge exchange processes as well.

In the energy range above 150-250 MeV, either JAM[8] or QMD[9] is employed for description of dynamical processes. For the statistical decay followed by the dynamical processes, the generalized evaporation model (GEM)[10] is incorporated. Both the frameworks have been demonstrated to reproduce well the measurements of double-differential nucleon and pion emission cross sections and fragment production cross sections for proton-induced reactions from 100 MeV up to 3 GeV.

In addition, the code TOTELA[11] based on systematics is used as a tool for evaluation of the total, elastic, and reaction cross sections for energies above 150-250 MeV The Niita systematics is used in TOTELA. For calculations of high-energy fission cross sections, the systematics-based code FISCAL[2] is applied. Furthermore, γ-ray energy spectra are calculated with the code ALICE-F[12].

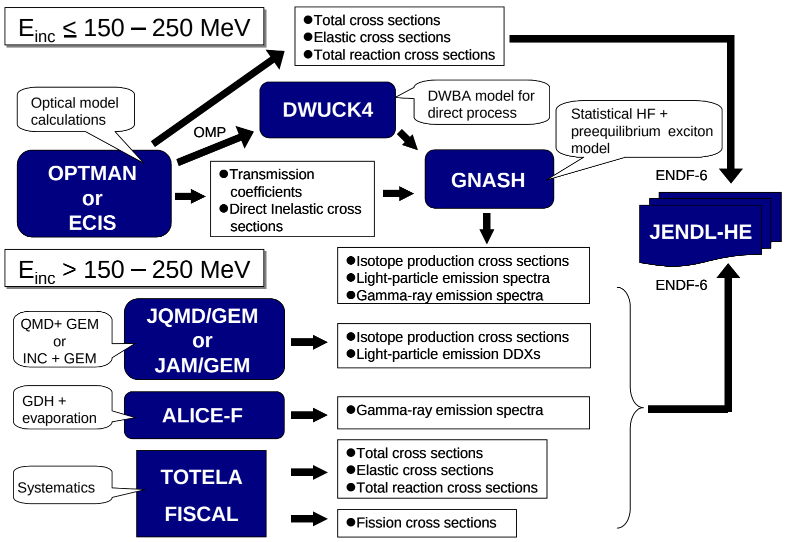

Fig.1 Nuclear model calculation code system used in the JENDL-HE evaluation

3. Results and comparisons with measurements and other evaluations

The cross sections were evaluated for nucleon-induced reactions on the nuclides listed in Table 1 using the above-mentioned model calculation codes. The evaluated cross sections are as follows: neutron total cross sections, nucleon elastic scattering cross sections and angular distributions, non-elastic cross sections, production cross sections and double-differential cross sections of secondary light particles (n, p, d, t, ^{3}He, α, and π) and γ-rays, isotope production cross sections, and fission cross sections. Neutron total cross sections and isotope production cross sections for several nuclei are evaluated using a fitting procedure of experimental data in the case where systematic measurements are available over a broad range of incident energy.

The present status of JENDL-HE file is as follows: the evaluations for 66 nuclides among the entire 132 nuclides have been completed as shown in Table 1, and the evaluated cross section data have been tabulated in the ENDF-6 format and released as the JENDL/HE-2004 file. For neutrons, the evaluated cross section data are merged with the data below 20 MeV taken from the JENDL-3.3[13]. For protons, the cross section data below 20 MeV are also included in the JENDL-HE. It should be noted that double-differential production cross sections of light particles are stored using the laboratory angle-energy law (LAW=7) of the ENDF-6 format.

Some representative results of the evaluated cross sections are shown below with experimental data and the other evaluations (LA150[1] and/or NRG2003[14]). Other results for the following elements are found elsewhere: C[15], Al[16], Mg and Si[17], K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni and Zn[18], Cu[19], Zr, Nb and W[20].

Neutron total cross sections and proton nonelastic cross sections for Fe is shown in **Fig. 2**. Three evaluations (JENDL-HE, LA150 up to 150 MeV, and NRG2003 up to 200 MeV) are in good agreement with experimental data[21]. Among them, the JENDL-HE data provide the largest values for neutron total cross sections over the whole energy range, and the smallest values for proton nonelastic cross sections in the energy range of 30-80 MeV.

The JENDL-HE result of angular distributions of neutron elastic scattering from ^{28}Si is compared with measurements[21] and the LA150 evaluation for nine incident energies in **Fig. 3**. Both the evaluations show excellent agreement with the experimental data to similar extent. As the incident energy increases, some differences between the JENDL-HE and the LA150 evaluations are seen at backward angles where there are no available experimental data.

Double-differential production cross sections of protons and deuterons are presented for proton-induced reactions on ^{12}C at 68 MeV in **Fig. 4**. For protons, both JENDL-HE and LA150 evaluations show good agreement with the experimental data[22]. For deuterons, some differences are obvious in both the evaluations, and the JENDL-HE is in better agreement with the measurement than the LA150 at 30 and 60 degrees. In **Fig. 5**, evaluated double-differential neutron production cross sections are compared with experimental data[23] for the (p,xn) reaction on ^{90}Zr at 120 MeV. The JENDL-HE evaluation is in fairly good agreement with the measurement in the continuum preequilibrium region, except for the Gamov-Teller (GT) resonance and the isobaric analog state (IAS) observed at 0 degree. The nuclear model codes used in the present evaluation are not capable of predicting such the resonance structure formed by direct charge-exchange processes.

Finally, an example of isotope production cross sections are shown in **Fig. 6**. The evaluated cross sections are compared with the experimental data[21] for ^{22}Na produced by the proton-induced reaction on ^{nat}Si. Both the JENDL-HE and LA150 evaluations reproduce the experimental data fairly well, although underestimation is seen for the LA150 at incident energies below 50 MeV.

4. Benchmark test

For validation of the evaluated cross sections, benchmark tests using the MCNPX transport code[24,25] were performed for neutron yields from stopping-length targets. Here, the preliminary result for carbon target bombarded by 113 and 256 MeV protons is shown in **Fig. 7** as an example. For 113 MeV, the MCNPX calculation using the JENDL-HE data shows excellent agreement with the measurement[26] except underestimation seen above 30 MeV at 7.5 degree, while the calculation using the LA150 data overestimates remarkably the measurement for neutrons between 3 and 20 MeV and underestimates it for neutrons above 30 MeV at 7.5 and 30 degrees. Both the MCNPX results with the JENDL-HE data and the LA150 data reproduce well the measurement[27] for 256 MeV protons to a similar extent, although overestimation is seen in the 5 to 20 MeV energy range at forward angles for the calculation with the LA150 data. It should be noted that the MCNPX calculation with the LA150 data is switched to the LAHET module automatically above 150 MeV.

5. Summary and conclusions

For the JENDL high-energy file (JENDL-HE), the cross sections were evaluated for neutrons and protons up to 3 GeV on the nuclides listed in Table 1, mainly on the basis of the nuclear model calculations and the systematics. The JENDL-HE evaluation were compared with the other evaluations and the experimental data, showing generally good agreement with them. Evaluations and compilations for the remaining 66 nuclides are underway. Further benchmark tests using transport codes, MCNPX and PHITS[28], are being performed for validation of the evaluated cross sections. Some preliminary results were partly reported. Through the benchmarks, revision and updating work will continue towards completion of the JENDL-HE file.

The current version of the JENDL-HE file does not contain information for heavy recoils (A > 4). Double-differential cross sections (DDXs) of all secondary ions are required for estimation of radiation effects in structural materials, microelectronic devices, and human bodies. Therefore, it will be our future task with high priority to provide reliable DDXs of heavy recoils and complex charged particles.

Acknowledgements

This work has been performed by the members of High-Energy File Making Sub-Working Group in High-Energy Nuclear Data Evaluation Working Group, JNDC. The author is deeply grateful to all the members for their cooperation and valuable discussions on the JENDL-HE evaluation.

References

[1] M.B. Chadwick, *et al*., *Nucl. Sci. Eng*., **131**, 293-328 (1999).
[2] T. Fukahori, *et al*., *J. Nucl. Sci. and Technol*., *Suppl.* **2**, 25-30 (2002).
[3] P.G. Young, *et al*., LA-12343-MS, Los Alamos National Laboratory (1992).
[4] H. Kalka, *et al*., *Z. Phys.*, **A341**, 289-299 (1992).
[5] J. Raynal, Proc. of a Specialists Meeting on Nucleon-Nucleus Optical Model Up To 200 MeV, Nov. 13-15, 1996, Buyères-le-Châtel, France, NEA Nuclear Science Committee, (1997), pp. 159-166.
[6] E.S. Sukhovitskiĩ, *et al*., OPTMAN and SHEMMAN codes, JAERI-Data/Code 98-019 (1998).
[7] P.D. Kunz and E. Rost, DWUCK4 code, *Computational Nuclear Physics 2: Nuclear Reactions*, (Springer-Verlag, Berlin, 1993, Eds. K. Langanke, et al.), pp. 88-107.
[8] Y. Nara, *et al*., *Phy. Rev. C* **61**, 024901 (2001).
[9] K. Niita, *et al*., *Phy. Rev. C* **52**, 2620-2635 (1995); JAERI-Data/Code 99-042 (1999).
[10] S. Furihata, *Nucl. Inst. Method in Phys. Res. B* **171**, 251-258 (2000); S. Furihata and T. Nakamura, *J. Nucl. Sci. and Technol. Suppl.* **2**, 758-761 (2002).
[11] T. Fukahori and K. Niita, *Summary Report of the Second Research Coordination Meeting on Nuclear Model Parameter Testing for Nuclear Data Evaluation (RIPL-II)*, June 12-16, 2000, Varenna, Italy, INDC(NDS)-416, pp.97 (2000).
[12] T. Fukahori, *Proc. of the Specialists' Meeting on High Energy Nuclear Data*, JAERI-M 92-039 (1992), pp.114-122.
[13] K. Shibata, *et al*., J. of Nucl. Sci. and Technol., **39**, 1125-1136 (2002).
[14] A.J. Koning, private communication (2004).
[15] Y. Watanabe, *et al*., presented at Int. Conf. on Nuclear Data for Science and Technology, Sept. 26- Oct.12, 2004, Santa Fe, USA; Proc. of the 2002 Nuclear Data Symp. JAERI-Conf 2003-006 (2003), pp.183-188.
[16] Y.O. Lee, *et al*., *J. Nucl. Sci. and Technol*., **36**, 1125-1134 (1999).
[17] W. Sun *et al*., presented presented at Int. Conf. on Nuclear Data for Science and Technology, Sept. 26-Oct.12, 2004, Santa Fe, USA.
[18] K. Kosako *et al*., presented presented at Int. Conf. on Nuclear Data for Science and Technology, Sept. 26-Oct.12, 2004, Santa Fe, USA.
[19] N. Yamano, *et al*., *Proc. of the 2002 Nuclear Data Symp*., JAERI-Conf 2003-006 (2003), pp.195-200.
[20] S. Kunieda, *et al*., *J. Nucl. Sci. and Technol*., **41**, 1033-1046 (2004).
[21] EXFOR, NEA Data Bank, URL http://www.nea.fr/html/dbdata.
[22] M. Harada, *et al*., *J. of Nucl. Sci. and Technol*., *Suppl.* **1**, 687-691 (2000); *J. of Nucl. Sci. and Technol*., *Suppl.* **2**, 393-396 (2002).
[23] W. Scobel, *et al*., *Phys. Rev. C* **41**, 2010-2020 (1990).
[24] H.G. Hughes, *et al*., *Proc. of the Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications*, Madrid, Spain, September 27-30, 1999, p.939; LA-UR-98-559 (1998).
[25] L.S. Waters(Ed.), MCNPX Uers's Manual, Version 2.3.0, LA-UR-02-2607 (2002).
[26] M.M. Meier, *et al*., *Nucl. Sci. Eng*., **102**, 310-321 (1989).
[27] M.M. Meier, *et al*., *Nucl. Sci. Eng*., **110**, 299-301 (1992).
[28] H. Iwasa, *et al., J. Nucl. Sci. and Technol*., **39**, 1142-1151 (2002).

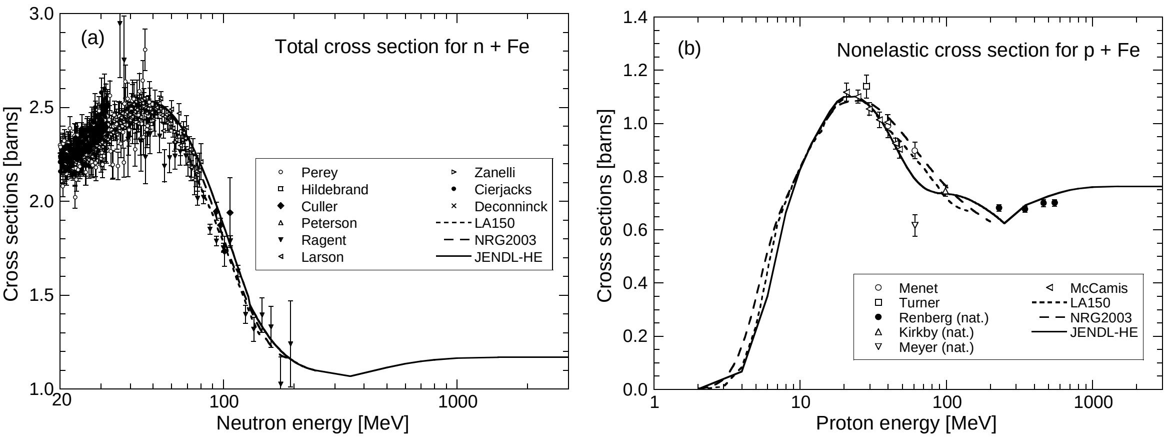

Fig.2 Neutron total cross section and proton nonelastic cross section for Fe

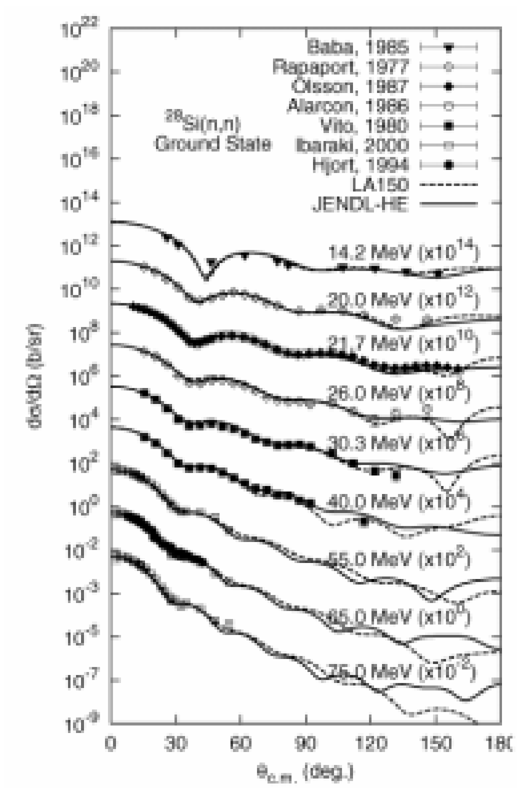

Fig.3 Angular distributions of neutron elastic scattering from ^{28}Si

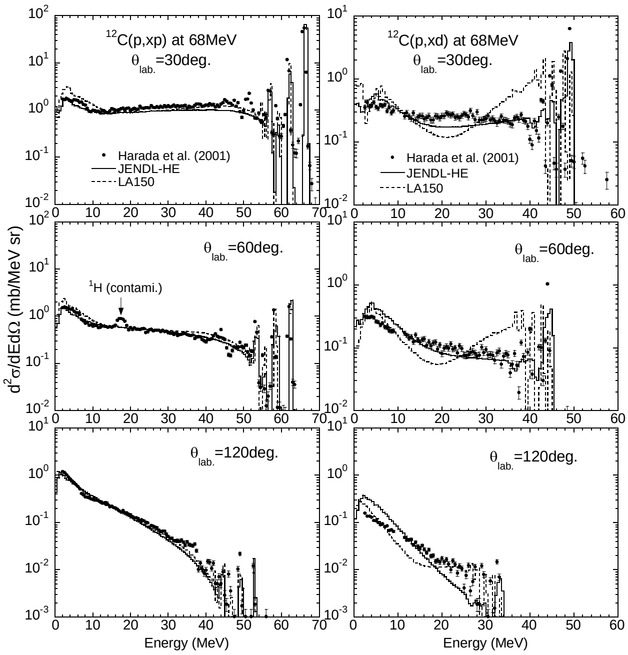

Fig.4 Double-differential proton and deuteron production cross-sections for proton-induced reactions on ^{12}C at 68 MeV

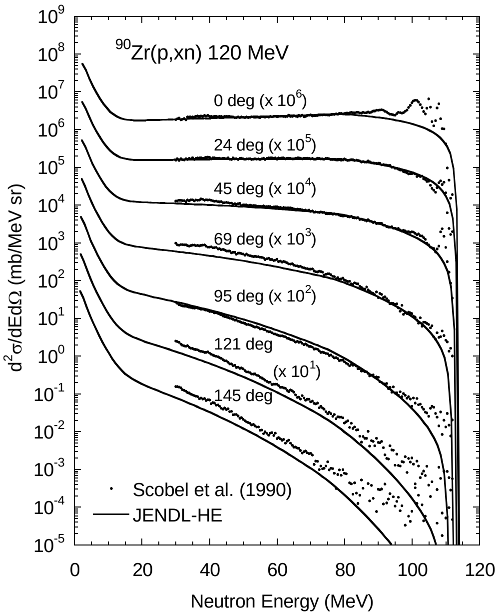

Fig.5 Double-differential neutron production cross sections for the ^{90}Zr(p,xn) reaction at 120 MeV

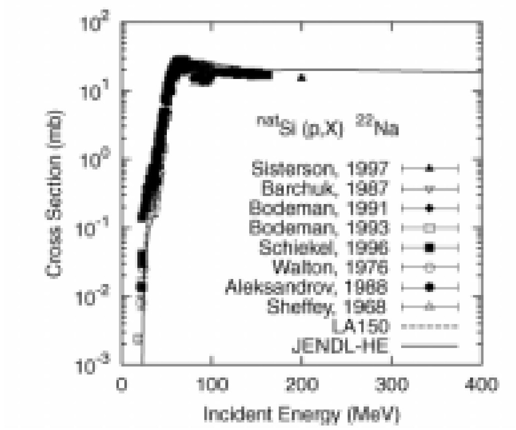

Fig.6 Production cross sections of ^{22}Na from the proton-induced reaction on ^{nat}Si

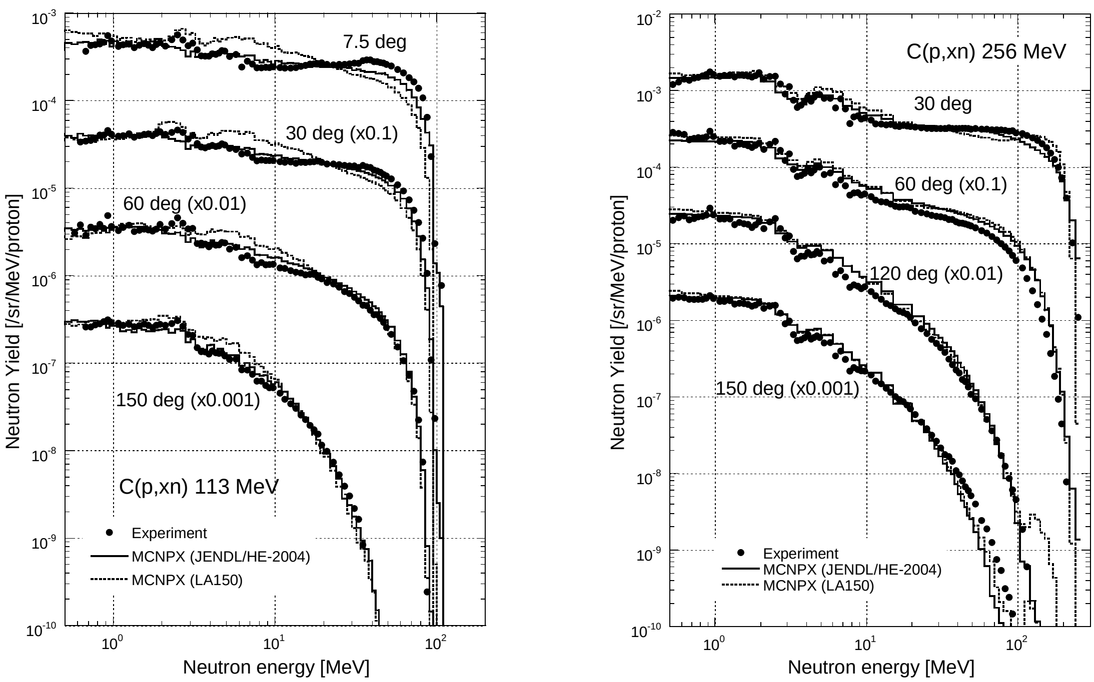

Fig.7 Comparison of MCNPX calculations and measurements for neutron yields from stopping-length carbon target for 113 MeV and 256 MeV protons.