The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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DEVELOPMENT OF VECTORIZED HIGH ENERGY MONTE CARLO CODE, MVP-JHET

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ABSTRACT

The three dimensional Monte Carlo code, MVP, has been used in the field of reactor design and shielding. The characteristics of MVP are the use of continuous energy cross sections and the vectorized coding of random walk. The vectorized MVP provides with fast calculation speed on a scalar computer. The MVP-JHET code was developed for high energy neutrons and protons based on MVP. It includes new functions of the high energy continuous cross section libraries, the treatment of transport and nuclear reaction by proton, and the scheme of intra-nuclear cascade by nucleon and meson. This is available to calculate neutron spectrum in the energy range from tens GeV to meV. The high energy library includes production cross section data of particles and mesons. The high energy neutron and proton libraries were produced from JENDL/HE-2004 and LA150. The transport process of proton was adopted the continuous slow down model, the stopping power by Barkas and Berger, and the method of pseudo collision. To verify MVP-JHET and its related libraries, three types of benchmark calculations were performed, and the results were compared with the experimental and calculated results. By using the libraries, the calculation speed was faster than other transport codes for high energy. The reliability of MVP-JHET was established by the present works.

Key Words: MVP, MVP-JHET, high energy transport, Monte Carlo

1 INTRODUCTION

In recent years, calculation methods and nuclear data in high energy region are required in advanced applications of accelerator engineering, cancer radiotherapy and space development. Various high energy calculation codes used a Monte Carlo method have been developed. Nuclear data for neutron and proton are especially important in these high energy applications. Neutron is important in high energy region also and variation of its energy is very large.

In order to realize fast and accurate Monte Carlo simulation of neutron and photon transport problems, the vectorized three-dimensional Monte Carlo code MVP [1] has been developed at JAERI. MVP is based on the continuous energy cross section model. Compared with conventional scalar codes, this code achieves higher computation speed by a factor of 10 or more on vector supercomputers. This has sufficient functions for production use by adopting accurate physics model, combination geometry description capability and variance reduction techniques. The first version was released in 1994 and has been extensively improved.

High energy transport calculation codes have been produced with various characteristics. In the past, the HETC [2], NMTC/JAERI [3] and LAHET [4] codes were used. These features were the Monte Carlo method, the empirical equation of cross section data and the nuclear cascade model. These codes were used many laboratories and had a lot of family codes. At present, the MCNPX [5], MARS [6] and PHITS [7] codes with Monte Carlo method are widely used in the world. MCNPX and PHITS are available the cross section library for MCNP [8] and some elementary particles of leptons, baryons and mesons. Computation speed of MARS is faster than MCNPX because of use of pseudo-cascade model.

Some evaluation works are underway to produce high energy evaluation file over 20 MeV for neutron and over threshold energy for proton. The LA150 file [9] is up to 150 MeV for 41 isotopes. The NRG2003 file [10] is up to 200 MeV for 26 isotopes. The JENDL/HE-2004 file [11, 12] is up to 3 GeV for 66 isotopes. These evaluated data are stored in the ENDF-6 format.

Because we must be treated the large energy variation for neutron (about 14 figures from tens GeV to meV) and the complicated geometry, useful and fast speed of a Monte Carlo code are necessary. Thus, the MVP-JHET code was developed for executing the transport calculation of high energy neutrons and protons based on MVP. MVP-JHET is also available the exclusive cross section library. We were investigated the benchmark calculation results.

2 MVP-JHET CODE

The three-dimensional high energy particle transport Monte Carlo code, MVP-JHET, was produced from MVP2. This is based on the FORTRAN 77 rule. Although this is vectorized, one is available on a normal scalar computer, too. The defined particles in MVP-JHET are neutron, photon, electron, proton, deuteron, triton, He-3, alpha, π^+, π^0, π^-, μ^+, μ^-, K^+, K^0_{long}, K^0_{short}, K^-, anti-proton, and anti-neutron. Currently, light ions (deuteron, triton, He-3 and alpha) aren’t available as transport particles. The defined particles have the particle identical number and all particles including baryons have also the special internal number.

The expanded terms of high energy transport used cross section library for MVP-JHET are as follows: (a) generation of particles including light ions, mesons and nucleon from neutron reaction, (b) treatment of proton reaction including particle generation, (c) free flight analysis of light ions, and (d) random walk control between particles. The transport process of proton and light ions was adopted the continuous slow down model, the stopping power by Barkas and Berger, and the method of pseudo collision.

The expanded terms of transport without library are as follows: (1) elastic scattering and nuclear reaction models [3], (2) Bertini model for intra-nuclear cascade reaction [3], (3) JAM model for defined particles and baryons [7], (4) statistical decay model (DRES, SDM, or GEM models) [3], (5) surface crossing tally, and (6) distinction of particles with/without library and connection energy depended on maximum energy of library. Although calculation without library is possible, reliability of neutron below tens MeV is very insufficient. The connection energy between JAM and Bertini models are set to 3.5 GeV for nucleon and 2.5 GeV for pion as default value, and other particles are used JAM only.

MVP-JHET runs on UNIX and Linux computers, and requires c shell and FORTRAN77 compiler as g77.

3 PRODUCTION OF CROSS SECTION LIBRARY

MVP-JHET can use both the general cross section libraries for MVP and the exclusive cross section libraries for high energy neutrons and protons. The general libraries consist ones for neutron incident, photon interaction and electron to approximate bremsstrahlung. The format of exclusive neutron library differs partly from the general neutron library and the exclusive proton library.

The merits by using a library are as follows: (i) computing efficiency is excellent and (ii) cross section data is explicit and the change is easy. The CPU time may be fast from few tens % to two times.

The MVP-JHET cross section library for high energy neutrons is produced by the LICEMH code and the proton library is done by the LICEMHP code. LICEMH and LICEMHP have been improved from the LICEM code [13] to produce the general neutron library. They process the evaluated nuclear data file for high energy neutrons and protons with ENDF-6 format. The nuclear data file has the form that all production cross section data are stored in MF=6/MT=5 section (proposed by LANL). In high energy region, evaluation is made only for production data of particles and nuclides, because emission processes of particles are indistinguishable.

The LA150 and JENDL/HE-2004 were processed by nuclides with LICEMH and LICEMHP, and the high energy neutron and proton cross section libraries for MVP-JHET were produced. The sizes of produced LA150 neutron and proton libraries are about 122 and 85 Mbytes with binary form. The processing conditions are as follows: precision of cross sections is 0.1%, temperature is 293.15 Kelvin for neutron, the number of equal-probability angular bins is 32, heating number is given to neutron only, and maximum energy is 150 MeV for LA150 and 3 GeV for JENDL/HE-2004 (JHE).

4 BENCHMARK CALCULATIONS

To verify MVP-JHET and its related libraries, three types of benchmark calculations were performed. The calculated results were compared with the experimental and other calculated ones.

4.1 WNR-LAMPF Experiment

The TTY (thick target yield) experiment at WNR-LAMPF facility in LANL was measured angular neutron energy spectra leaked from cylindrical targets by TOF method.[14] The energies of incident protons are 113 and 256 MeV.

This benchmark calculation is performed by MVP-JHET and MCNPX. The leakage neutron spectra from carbon targets were shown in Figs. 1 to 3. Fig. 1 is compared JHE and LA150 libraries by MVP-JHET for 113 MeV proton, and Figs. 2 and 3 are done MVP-JHET and MCNPX by JHE library for 113 and 256 MeV protons. The results of MVP-JHET are good agreement with the experiment and MCNPX. The result of carbon in JHE agrees completely, but 113 MeV of LA150 is inappropriate.[11] Figs. 4 and 5 are the comparison between MVP-JHET and MCNPX by LA150 for iron targets irradiated by 113 and 256 MeV protons. The results of iron targets agree almost, but Fig. 5 is shown neutron spectra by internal cross section data in codes because 256 MeV proton is exceeded the upper energy of LA150.

These CPU times are shown in Table I. The CPU time of MVP-JHET is faster 2 to 10 times than MCNPX in this calculation model. The CPU of scalar computer is Pentium IV 3 GHz, the memory is 1 GB and the OS is RedHat9 Linux.

Table I. The CPU times of TTY experiment at WNR/LAMPF in LANL (Pentinum IV 3 GHz).

target	proton		library	code	CPU time [min]
	energy [MeV]	number of sources			
carbon	256	1.00E+08	LA150	MCNPX	5097
				MVP-JHET	568
			JENDL/HE-2004	MCNPX	4920
				MVP-JHET	38
	113		LA150	MCNPX	1330
				MVP-JHET	21
			JENDL/HE-2004	MCNPX	1090
				MVP-JHET	20
iron	256	1.00E+08	LA150	MCNPX	10770
				MVP-JHET	507
	113			MCNPX	3068
				MVP-JHET	41

4.2 TIARA Iron Penetration Experiment

The penetration experiment at TIARA facility in JAERI was measured leakage neutron spectra from iron shielding assembly irradiated neutrons that generated by ^{7}Li(p,n) reaction.[15] The size of iron assembly is 120x120xT [cm^{3}], and the thickness (T) are 20, 40, 70, 100 and 130 cm. The energies of incident protons are 43 and 68 MeV. The source spectra used to calculations are the quasi-monoenergetic source neutrons from ^{7}Li targets bombarded proton and they were obtained by measurements.

Figs. 6 and 7 are the leakage neutron spectra from 40 and 130 cm-thicknesses of irons for 68 MeV protons. The results of MVP-JHET and MCNPX used same LA150 agree in 40 cm-thickness, but the 130 cm-thickness of results overestimate. For deep penetration of iron over 70 cm-thicknesses, JHE is better than LA150. The jagged peaks between 30 and 60 MeV of MVP-JHET in Fig. 7 are the cause of linear-linear interpolation for energy-angle distributions of neutron production in LA150.

4.3 AGS Experiments

The two kinds of high energy experiments at AGS facility in BNL was performed under the collaborative program of JAERI and BNL.[16]

4.3.1 Activation reaction rate distribution on a mercury target

The activation reaction rate was measured on axis direction around a mercury target bombarded by 1.6, 12 and 24 GeV protons. The size of cylindrical mercury target is 20 cm-diameter and 130 cm-length. Measured reaction rates are In-115(n,n')In-115m, Al-27(n,x)Na-23, and Bi-209(n,4n)Bi-206.

Figs. 8 to 10 are the comparison between MVP-JHET and MCNPX with JENDL-3.3 library below 20 MeV for three reactions. MCNPX is 1.6 GeV proton only. The results of Al-27 and In-115 are as well as the experiment. Bi-209 is underestimated tens % to half times than experiment. It was verified that MVP-JHET could have the calculation capability up to 24 GeV.

4.3.2 Deep penetration on steel and concrete

The activation reaction rate was measured in the steel and concrete shielding regions surrounded the target room including above mercury target. The energies of incident protons are 2.83 and 24 GeV.

Figs. 11 and 12 for 2.83 GeV protons are reaction rates of In-115 and Al-27 in the steel and concrete regions calculated by MVP-JHET with JENDL-3.3 library. In-115 agrees within tens % with the experiment and Al-27 does within factor 2. Figs. 13 and 14 for 24 GeV are those of In-115 and Bi-209. Those in steel are good agreement with experiment and in concrete are agreement within factor 2.

5 SUMMARY

We developed the vectorized high energy Monte Carlo code, MVP-JHET. This treats particles of neutron, proton, photon, mesons and baryons. This is available to calculate in the neutron energy range from tens GeV to meV and the upper energy of other particles is tens GeV. The high energy neutron and proton libraries were produced from JENDL/HE-2004 and LA150.

To verify MVP-JHET and its related libraries, three types of benchmark calculations were carried out. The consistency between MVP-JHET and MCNPX results was confirmed and the agreement between MVP-JHET and experiment was estimated. Thus, the reliability of MVP-JHET was established. The calculation speed by using a library is compared with MCNPX and the fast capability is specified.

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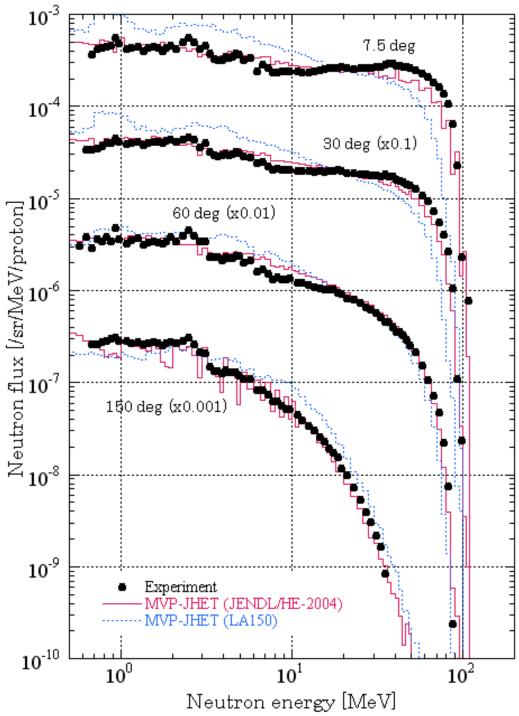

Figure 1. Angular neutron spectra by MVP-JHET from C target irradiated by 113 MeV protons at WNR.

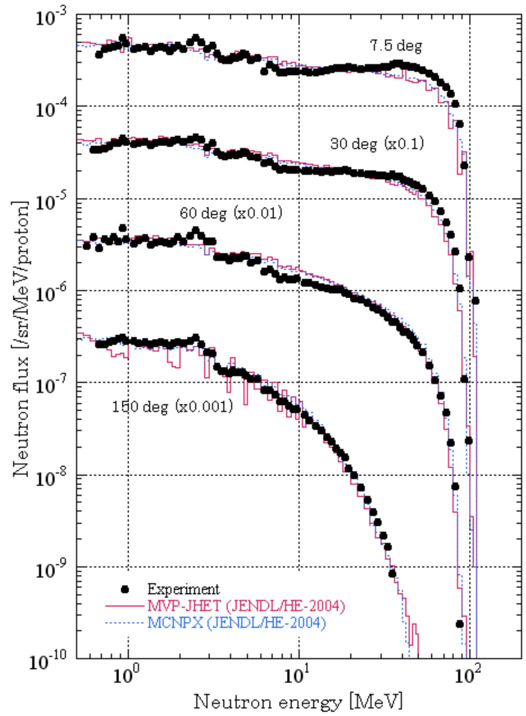

Figure 2. Angular neutron spectra by MVP-JHET and MCNPX from C target irradiated by 113 MeV protons at WNR.

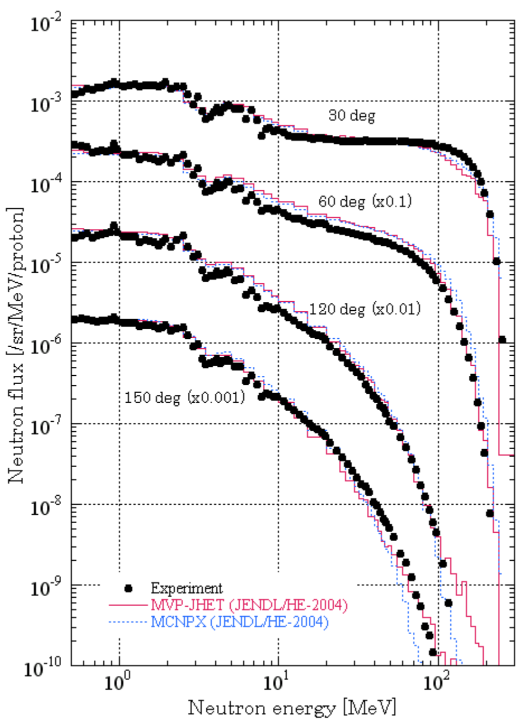

Figure 3. Angular neutron spectra by MVP-JHET and MCNPX from C target irradiated by 256 MeV protons at WNR.

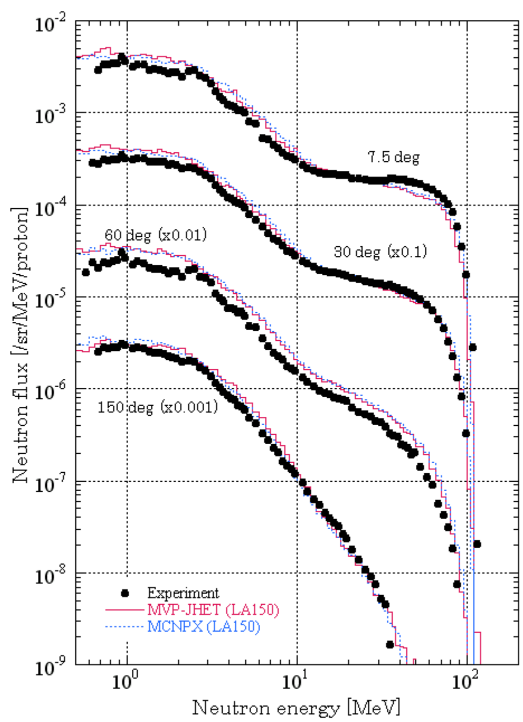

Figure 4. Angular neutron spectra by MVP-JHET and MCNPX from Fe target irradiated by 113 MeV protons at WNR.

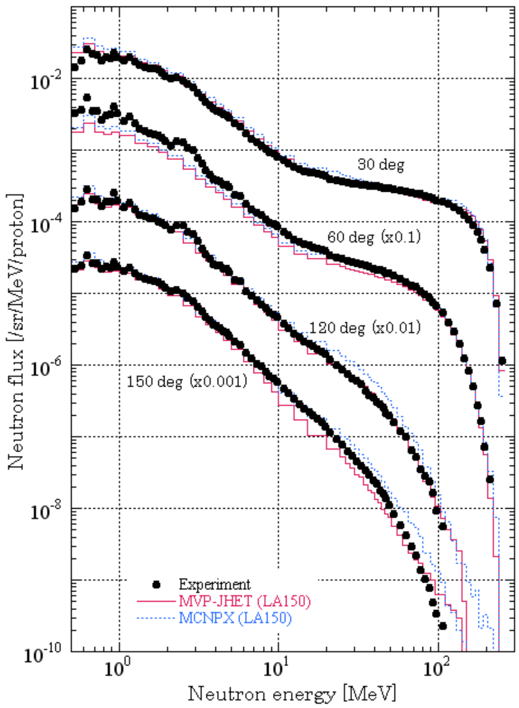

Figure 5. Angular neutron spectra by MVP-JHET and MCNPX from Fe target irradiated by 256 MeV protons at WNR.

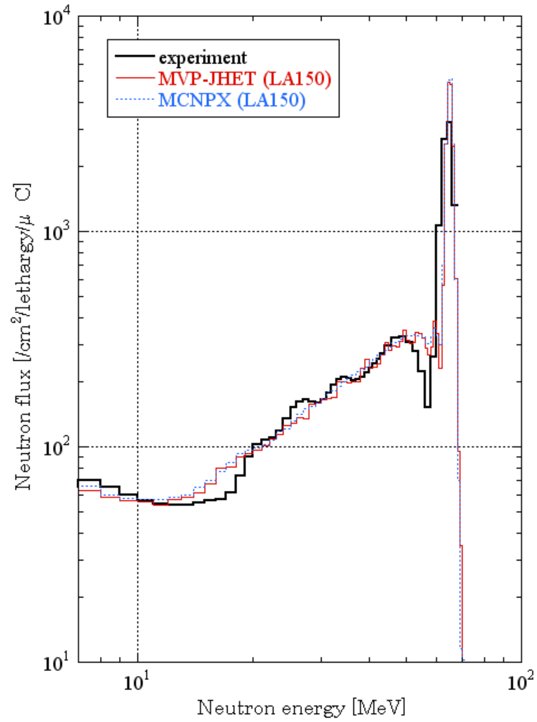

Figure 6. Leakage neutron spectra on beam axis from Fe 40 cm assembly irradiated by neutrons of p_^{7}Li at TIARA.

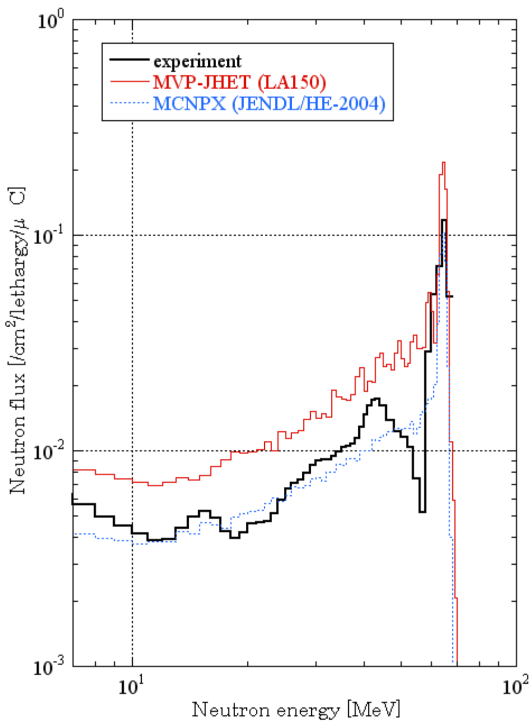

Figure 7. Leakage neutron spectra on beam axis from Fe 130 cm assembly irradiated by neutrons of p_^{7}Li at TIARA.

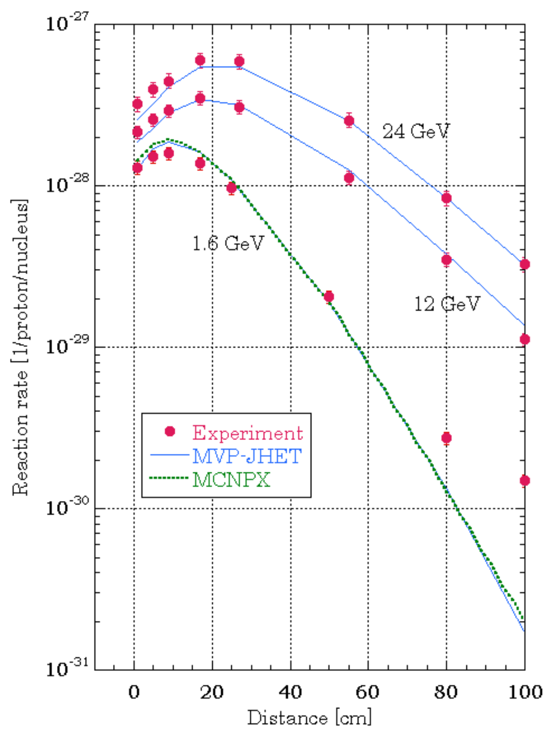

Figure 8. ^{27}Al(n,x)^{24}Na reaction rates on axis direction around mercury target bombarded by protons at AGS.

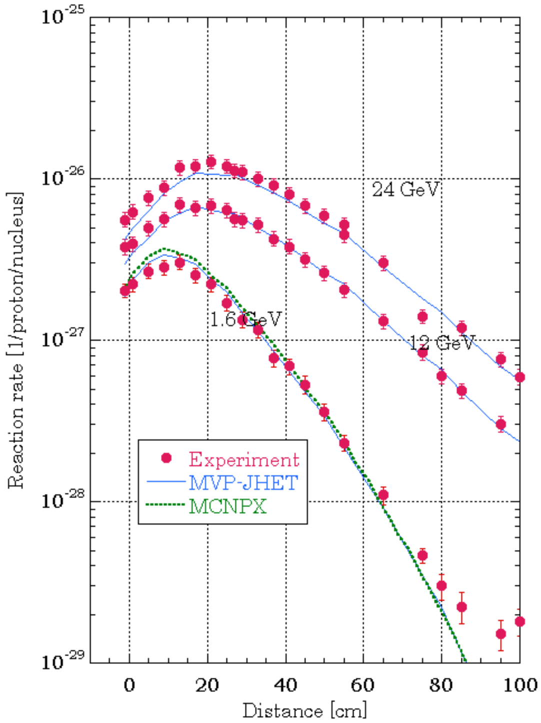

Figure 9. $^{115}In(n,n')^{115m}In$ **reaction rates on axis direction around mercury target bombarded by protons at AGS.**

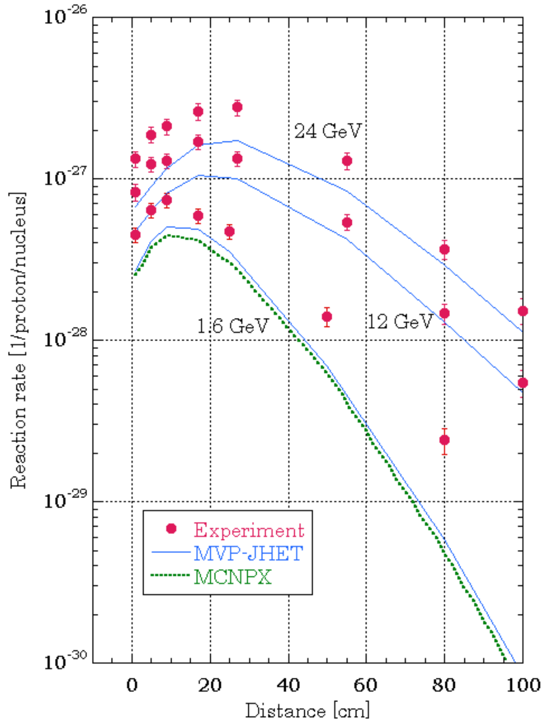

Figure 10. $^{209}Bi(n,4n)^{206}Bi$ **reaction rates on axis direction around mercury target bombarded by protons at AGS.**

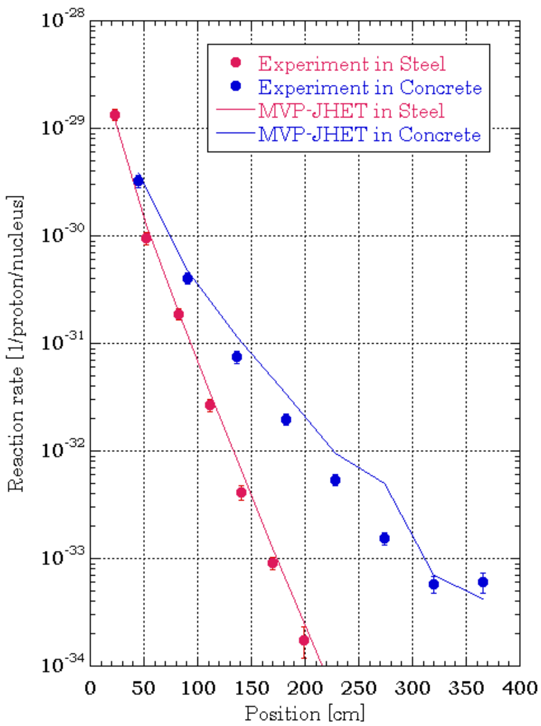

Figure 11. $^{115}In(n,n')^{115m}In$ **reaction rates in steel and concrete by neutrons from mercury target bombarded by 2.83 GeV protons at AGS.**

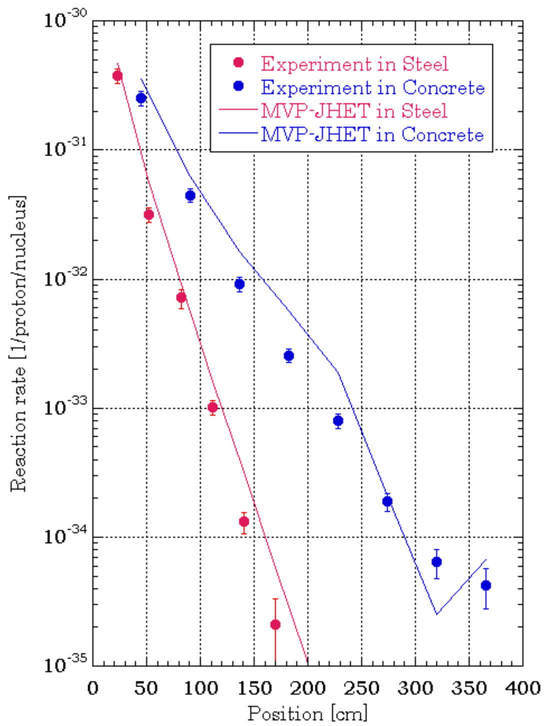

Figure 12. $^{27}Al(n,x)^{24}Na$ **reaction rates in steel and concrete by neutrons from mercury target bombarded by 2.83 GeV protons at AGS.**

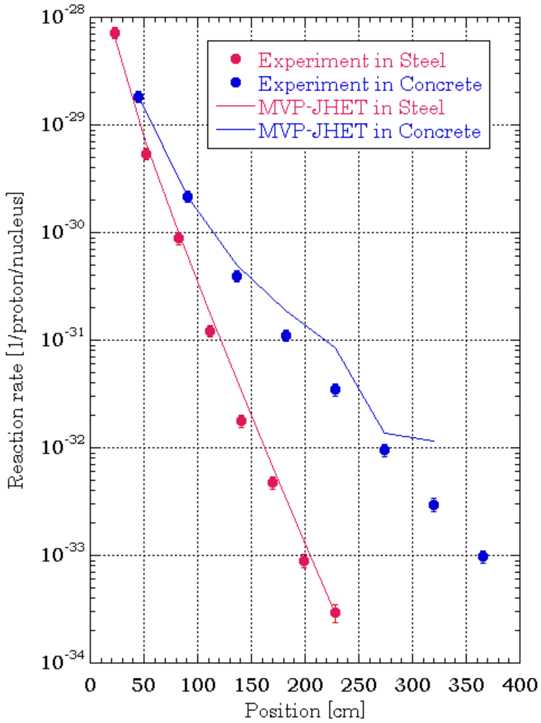

Figure 13. ^{115}In(n,n')^{115m}In reaction rates in steel and concrete by neutrons from mercury target bombarded by 24 GeV protons at AGS.

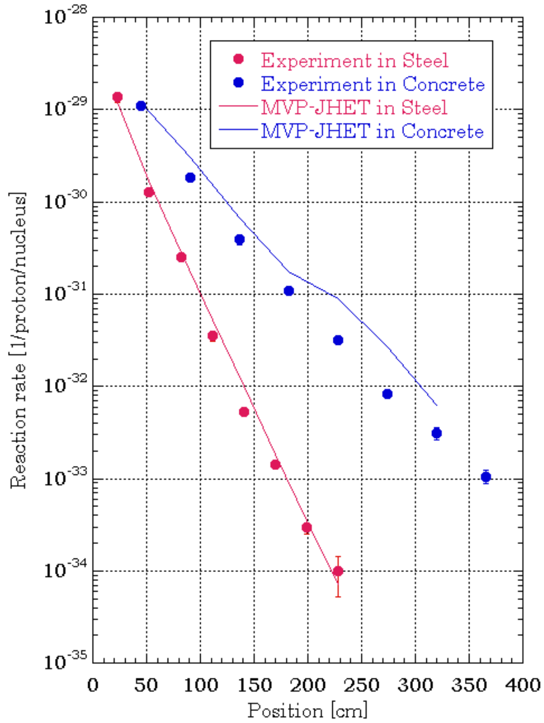

Figure 14. ^{209}Bi(n,4n)^{209}Bi reaction rates in steel and concrete by neutrons from mercury target bombarded by 24 GeV protons at AGS.