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Status of the MCNP™/LCS™ Merger Project

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ABSTRACT

The MCNPX code is now in limited release in a beta-test version. We provide a brief status report on the physics modules now in the code and of the enhanced capabilities to use new evaluated neutron data. We also present new benchmark calculations in which LAHET and MCNPX are compared with experimental results from the Japan Atomic Energy Research Institute.

1. INTRODUCTION

A major code-development effort is underway at Los Alamos National Laboratory, primarily in support of the computational needs of the Accelerator Production of Tritium (APT) program. Emphasis of the project is twofold: (1) merging existing functionality of the MCNP† code[1] and the LAHET Code System (LCS);[2] and (2) improving the physics capabilities of the merged code. A prototype of the expanded code, called MCNPX, was released about one year ago,[3] and intermediate versions have been presented in several venues.[4–5] A preliminary beta-test version, MCNPX Version 2.1.2, is now in limited release for testing. We anticipate the release of a production version of MCNPX during FY98.

The starting point for the code merger effort was MCNP Version 4B. MCNPX expands the capabilities of MCNP by increasing the set of transportable particles,[6] by making use of newly evaluated high-energy nuclear data tables for neutrons,[7] and by incorporating physics models for use where tabular data are unavailable. All of the LAHET nuclear physics modules are included intact in MCNPX, which expands the capabilities of LAHET through the availability of many of the variance reduction methods of MCNP, and through the incorporation of MCNP's very general syntax for specifying geometry, sources, and tallies.

The MCNPX code development has been managed in a modular fashion, so that the future inclusion of additional physics models will be straightforward. Recent emphasis has been on improving existing models for collisional energy-loss processes and angular deflection for charged particles, and on implementing the capability to use newly-evaluated high-energy nuclear data tables for incident protons.[8] The result of this project will be a unified, general Monte Carlo transport capability to model a fully-coupled cascade of nuclear particles over a wide energy range.

2. PHYSICS MODULES

2.1 CHARGED-PARTICLE TRANSPORT

For charged particles other than electrons, the collisional energy-loss (stopping power) model has been improved, and now consists of a modified Bethe-Bloch formulation above 1.3 MeV/AMU, and the model from the SPAR[9] code currently used in LAHET below 2.6 MeV/AMU. The two models are interpolated in energy over the range between 1.3 and 2.6 MeV/AMU.

In the high energy range the Bethe equation is used without approximation, which provides a more accurate treatment for muon and pion calculations than has been the practice to date with SPAR (and LAHET). The principal corrections applied are the shell correction model of Janni[10] and the density (or polarization) effect correction of Sternheimer,[11] the latter in a more detailed form than used in LAHET. Following Janni, a small correction introduced

† LAHET, MCNP, and MCNPX are trademarks of the Regents of the University of California, Los Alamos National Laboratory.

by the second Born approximation is included, although it has very small effect. The adjusted ionization potentials are those of Berger and Seltzer[12] as given in ICRU Report 37.[13] At the present time, the stopping power model at low energies, below 2.6 MeV/AMU, has been taken directly over from the LAHET code. The model, originally developed for the SPAR code, is based on the methods of Linhard[14–15] and includes a nuclear stopping power model for very low energies. There is no low-energy cutoff in the calculation. The effective charge treatment is that of Barkas.[16]

These new procedures provide a small but significant improvement over LAHET practice above 1 MeV/AMU, especially for muon and pion transport, while offering a smoother and more reliable transition to the low energy model.

A small-angle Coulomb scattering treatment, absent in earlier versions of MCNPX, has been added to the new release. We use a Gaussian model based on a theory presented by Rossi. In the original theory, both angular deflections and small spatial displacements were accounted for. Since the complex geometric system of MCNP (and therefore MCNPX) does not yet accommodate transverse displacements in charged-particle substeps, we use only the part of the theory that addresses the angular deflection. In several test cases, this slight approximation has been found to have negligible effects on the results.

Finally, the charged-particle energy-loss straggling is sampled using a prototype implementation[17] of the Vavilov theory. This module is expected to be updated or replaced in a future version of the code.

2.2 OTHER PHYSICS MODULES

MCNPX incorporates all of the basic LAHET nuclear physics modules. These include the Bertini[18] and ISABEL[19-20] intranuclear cascade (INC) models, the multistage pre-equilibrium exiton model,[21] the evaporation model,[22] the ORNL[23] (Oak Ridge National Laboratory) and RAL[24] (Rutherford Appelton Laboratory) models for fission induced by high-energy interactions, the Fermi breakup model,[25] the nucleon elastic scattering model,[26] and the gamma production[2] (PHT) models. A version of the FLUKA[27] high-energy generator is also included. The particle decay features of LAHET are also present in their entirety. Transport cross sections, where not determined by MCNPX library methods, are defined as in LAHET. The LAHET data files BERTIN and PHTLIB are now accessed by MCNPX to provide the necessary data for the included LAHET modules.

3. EVALUATED PARTICLE-PRODUCTION DATA

An important requirement of the current code- and data-development plan is to develop the necessary tools to model transport of coupled neutral and charged particles below 150 MeV based on nuclear-data evaluations. This release of MCNPX partially meets that requirement. The physics capabilities of MCNP have been upgraded[28] to include the production of secondary charged particles from neutron collisions, using data contained on expanded continuous-energy neutron cross-section tables.

The ENDF6 format[29] allows nuclear-data evaluators to include explicitly multiplicities and spectra of charged particles resulting from neutron reactions. Recently, Chadwick and Young have produced several such evaluations,[8] fully utilizing the "n-particle" capabilities of the ENDF6 format, and also extending the energy range of the incident particle to 150 MeV.

An expanded format for MCNP continuous-energy data tables, to permit an arbitrary number of secondary-particle species, has been developed. An auxiliary processing code called ADDCP has been written to create MCNP data tables in this expanded format. The current neutron-data library resulting from these efforts contains cross-section tables for 15 isotopes, and is described in Ref. 30.

In order to use these new evaluations and the corresponding data tables, the routines in MCNP for reading cross sections and for sampling secondary particles have been expanded. The modifications have been managed so that the methods applicable to neutron-induced charged-particle production are very similar to the existing methods for neutron-induced photon production. As in the existing neutron-induced photon algorithm, the code performs a significant amount of pre-transport data manipulation. In particular, the list of active particle types for a given problem (specified on the MODE card) is used to expunge unneeded data for the problem. Neutron heating numbers are also modified based on the charged particles to be transported.

At every neutron collision, the possibility exists to produce secondary charged particles. All data used in the sampling process are specific to the collision isotope, and are evaluated at the incident neutron energy. The expected weight of a particular charged particle i is

$$\mathrm{WGT} \cdot \sigma_{\mathrm{cp},\, i}(E) / \sigma_{\mathrm{tot}}(E) \ ,$$

where WGT is the weight of the incident neutron, $\sigma_{\mathrm{cp},\, i}$ is the total particle-production cross section, σ_{tot} is the total neutron-interaction cross section, and E is the incident neutron energy. The number of charged particles produced is an integer (possibly 0) determined by analog sampling. If the code determines that a charged particle will be produced, it then samples the reaction responsible for that particle. There is no correlation between the type of neutron collision and the reactions sampled as being responsible for the various secondary particles that may be produced.

MCNPX supports several ENDF6 representations of scattered energy-angle distributions. Specifically, the following representations for secondary charged particles are allowed: tabular energy distributions; angular distributions via equally-probable cosine bins; Kalbach systematics for correlated energy-angle distributions; discrete two-body scattering; and n-body phase-space energy distributions. In all cases where necessary, kinematics algorithms currently incorporated in MCNP, which are specific for (*neutron-in, neutron-out*) physics, have been generalized to the (*neutron-in, charged-particles-out*) situation. In addition, a general center-of-mass to laboratory conversion technique has been incorporated based on Ref. 31. As is currently the case for neutron production, all such conversions are based on the assumption of two-body kinematics, which is clearly only an approximation for many high-energy neutron reactions of current interest.

4. NEW EXPERIMENTAL BENCHMARKS

A number of basic quality assurance tests have been performed for MCNPX. These include the standard set of MCNP test problems,[32] and a variety of problems created to ensure internal consistency of the code and agreement with the new data evaluations. There tests have been described in References 3 and 30. Here we present new benchmark calculations comparing both LAHET and MCNPX with experiments performed at the Japan Atomic Energy Research Institute (JAERI).

A number of neutron transmission experiments have been performed at the Azimuthally Varying Field Cyclotron facility at the JAERI Takashi site. These experiments are described in two published papers[33–34] and in two JAERI reports.[35–36] Briefly, incident 43- or 68-MeV protons impinged on converters consisting of 99.9% enriched ^{7}Li. The ^{7}Li(p,n) reaction produced nearly monoenergetic neutrons, which were then collimated and allowed to strike iron or concrete targets of various thicknesses. The neutron transmission was measured at several positions relative to the transmission target. Although the neutrons were initially almost monoenergetic in all cases, their actual spectra were measured in order to allow for more realistic comparison with neutron transport calculations.

Before MCNPX was available, simulations of some of these experiments were performed by Hertel and Evans using LCS. Reference 37 describes their calculations in detail, and for completeness, includes sample LAHET and MCNP input files. Calculations were performed using LAHET version 2.7 and version 2.8, which includes a new elastic scattering model[26] for neutrons above 15 MeV and for protons above 50 MeV. The conclusion of the investigation was that simulations using LAHET version 2.8 were in markedly better agreement with experiment than were simulations done with LAHET version 2.7, but that substantial systematic errors remained.

We have now repeated some of Hertel and Evans' calculations using MCNPX, replacing the LAHET transport model with the use of the new evaluated neutron data tables throughout the energy range of the experiments. Specifically, we have calculated the transmission of the quasi-monoenergetic 68-MeV neutron source through 40 cm of iron, and predicted the fluence on-axis and at 20 cm and 40 cm off-axis, for detectors immediately adjacent to the downstream face of the transmission target. In Fig. 1–3, we compare the experimental results with the previous calculations using LAHET versions 2.7 and 2.8 and with the new MCNPX results. In all cases, there is a dramatic improvement in agreement with the MCNPX calculations using the new evaluated neutron data tables.

5. CONCLUSION

Development of the MCNPX code, combining the capabilities of LAHET and MCNP, and enabling the use of newly available data, is proceeding apace. The new code is already providing improved simulations of experimental benchmarks.

REFERENCES

1. Judith F. Briesmeister, Editor, "MCNP™ — A General Monte Carlo N–Particle Transport Code," Los Alamos National Laboratory Report LA–12625–M, Version 4B (March 1997).
2. Richard E. Prael and Henry Lichtenstein, "User Guide to LCS: The LAHET Code System," Los Alamos National Laboratory Report LA–UR–89–3014, Revised (September 15, 1989). Also available at the World Wide Web site *http://www-xdiv.lanl.gov/XTM/lcs/lahet-doc.html.*
3. H. Grady Hughes, Richard E. Prael, and Robert C. Little, "MCNPX — The LAHET/MCNP Code Merger," Los Alamos National Laboratory Report XTM–RN(U)97–012, April 22, 1997.
4. H. Grady Hughes, Kenneth J. Adams, Mark B. Chadwick, Jack C. Comly, Stephanie C. Frankle, John S. Hendricks, Robert C. Little, Richard E. Prael, Laurie S. Waters, and Phillip G. Young, Jr., "MCNPX™ —The LAHET™/MCNP™ Code Merger," in *Proceedings of the Third Workshop on Simulating Accelerator Radiation Environments (SARE3)*, KEK Proceedings **97–5** (June 1997) 44.
5. H. G. Hughes, Kenneth J. Adams, Mark B. Chadwick, Jack C. Comly, Stephanie C. Frankle, John S. Hendricks, Robert C. Little, Richard E. Prael, Laurie S. Waters, and Phillip G. Young, Jr., "The MCNP™/LCS™ Merger Project," in *Topical Meeting on Nuclear Applications of Accelerator Technology,* American Nuclear Society Proceedings (Albuquerque, NM, November 1997) 213.
6. H. Grady Hughes and Laurie S. Waters, "Many-Particle MCNP," Los Alamos National Laboratory technical memorandum XTM:*96–91* (U) February 29, *1996.*
7. Robert C. Little, Stephanie C. Frankle, H. Grady Hughes, and Richard E. Prael, "Utilization of New 150-MeV Neutron and Proton Evaluations in MCNP," to be published in *Proceedings of the International Conference on Nuclear Data for Science and Technology,* Trieste, Italy (May 1997).
8. Phillip G. Young and Mark B. Chadwick, "Neutron- and Proton-Induced Nuclear Data Libraries to 150 MeV for Accelerator-Driven Applications," to be published in *Proceedings of the International Conference on Nuclear Data for Science and Technology,* Trieste, Italy (May 1997).
9. T. W. Armstrong and K. C. Chandler, "SPAR, A Fortran Program for Computing Stopping Powers and Ranges for Muons, Charged Pions, Protons, and Heavy Ions," Oak Ridge National Laboratory Report ORNL–4869 (May 1973).
10. Joseph F. Janni, *Atomic and Nuclear Data Tables* **27** (1982) 147–339.
11. R. M. Sternheimer and R. F. Peirls, *Phys. Rev. B* **3**, (1971) 3681.
12. M. J. Berger and S. M. Seltzer, National Bureau of Standards Report NBSIR 82–2550–A (1983).
13. ICRU (International Commission of Radiation Units and Measurements) Report 37 (1984).
14. J. Linhard and M. Scharff, "Energy Loss in Matter by Fast Particles of Low Charge", *Dan. Mat. Fys. Medd.* **27**, no. 15 (1953).
15. J. Linhard, M. Scharff, and H. E. Schiott, "Range Concepts and Heavy Ion Ranges," *Dan. Mat. Fys. Medd.* **33**, no. 14 (1963).
16. Walter H. Barkas, *Nuclear Research Emulsions, Vol. 1,* Academic Press, New York, 1963, p. 372.
17. H. Grady Hughes and Laurie S. Waters, "Energy Straggling Module Prototype," Los Alamos National Laboratory technical memorandum XTM:95–305 (U) November 29, 1995.
18. H. W. Bertini, *Phys. Rev.* **188** (1969) 1711.
19. Y. Yariv and Z. Fraenkel, *Phys. Rev. C* **20** (1979) 2227.
20. Y. Yariv and Z. Fraenkel, *Phys. Rev. C* **24** (1981) 488.

21. R. E. Prael and Michael Bozoian, "Adaptation of the Multistage Pre-equilibrium Model for the Monte Carlo Method (I)," Los Alamos National Laboratory Report LA–UR–88–3238 (September 1988).

22. L. Dresner, "EVAP — A Fortran Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei," Oak Ridge National Laboratory Report ORNL–TM–7882 (July 1981).

23. J. Barish, T. A. Gabriel, F. S. Alsmiller, and R. G. Alsmiller, Jr., "HETFIS High-Energy Nucleon-Meson Transport Code with Fission," Oak Ridge National Laboratory Report ORNL–TM–7882 (July 1981).

24. F. Atchison, "Spallation and Fission in Heavy Metal Nuclei under Medium Energy Proton Bombardment," in *Targets for Neutron Beam Spallation Sources*, Jül–Conf–34, Kernforschungsanlage Jülich GmbH (January 1980).

25. D. J. Brenner, R. E. Prael, J. F. Dicello, and M. Zaider, "Improved Calculations of Energy Deposition from Fast Neutrons," in *Proceedings, Fourth Symposium on Neutron Dosimetry*, EUR–7448, Munich–Neuherberg (1981).

26. R. E. Prael and D. G. Madland, "LAHET Code System Modifications for LAHET2.8," Los Alamos National Laboratory Report LA–UR–95–3605 (September 1995).

27. P. A. Aarnio *et. al.*, "FLUKA89," Consiel Europeene Organisation pour La Recherche Nucleaire Informal Report (January 2, 1990).

28. Robert C. Little, "MCNP Patch to Utilize Neutron-Induced Charged-Particle Data," Los Alamos National Laboratory technical memorandum XTM:97–73 (U) March 28, 1997.

29. V. McLane, C. L. Dunford and P. F. Rose, Editors, "ENDF–102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF–6," BNL–NCS–44945 Revised (November 1995).

30. Robert C. Little, "APT Neutron Library for MCNP — Version 1," Los Alamos National Laboratory Report XTM–RN(U)97–026, July 25, 1997.

31. R. E. Seamon, "Revision to ENDF–102 for the Kalbach–87 Distribution," Los Alamos National Laboratory technical memorandum X–6:RES–93–68 (January 27, 1993).

32. Ronald C. Brockhoff and John S. Hendricks, "A New MCNP™ Test Set," Los Alamos National Laboratory Report LA–12839 (September 1994).

33. Noriaki Nakao, Hiroshi Nakashima, Takashi Nakamura, Shun-ichi Tanaka, Sumusu Tanaka, Kazuo Shin, Mamoru Baba, Yukio Sakamoto, and Yoshihiro Nakane, "Transmission Through Shields of Quasi-Monoenergetic Neutrons Generated by 43- and 68-MeV Protons —I: Concrete Shielding Experiment and Calculation for Practical Application," *Nuclear Science and Engineering* **124**, No. 2 (October 1996) 228.

34. Hiroshi Nakashima, Noriaki Nakao, Shun-ichi Tanaka, Takashi Nakamura, Kazuo Shin, Sumusu Tanaka, Hiroshi Takada, Shin-ichiro Meigo, Yoshihiro Nakane, Yukio Sakamoto, and Mamoru Baba, "Transmission Through Shields of Quasi-Monoenergetic Neutrons Generated by 43- and 68-MeV Protons —II: Iron Shielding Experiment and Analysis for Investigating Calculational Method and Cross-Section Data," *Nuclear Science and Engineering* **124**, No. 2 (October 1996) 243.

35. Hiroshi Nakashima, Noriaki Nakao, Shun-ichi Tanaka, Takashi Nakamura, Kazuo Shin, Sumusu Tanaka, Shin-ichiro Meigo, Yoshihiro Nakane, Hiroshi Takada, Yukio Sakamoto, and Mamoru Baba, "Experiments on Iron Shield Transmission of Quasi-Monoenergetic Neutrons Generated by 43- and 68-MeV Protons via the ^{7}Li(p,n) Reaction," Japan Atomic Energy Research Institute, JAERI–Data/Code 96–005 (March 1996).

36. Yoshihiro Nakane, Katsumi Hayashi, Yukio Sakamoto, Nobuaki Yoshizawa, Noriaki Nakao, Syuichi Ban, Hideo Hirayama, Yoshitomo Uwamino, Kazuo Shin, and Takashi Nakamura, "Neutron Transmission Benchmark Problems for Iron and Concrete Shields in Low, Intermediate and High Energy Proton Accelerator Facilities," Japan Atomic Energy Research Institute, JAERI–Data/Code 96–029 (September 1996).

37. Nolan E. Hertel and Thomas M. Evans, "Benchmarking the LAHET Elastic Scattering Model for APT Design Applications," ERDA Final Report, Prepared for the Westinghouse Savannah River Company under ERDA Task Order 96-081 (August 14, 1997).

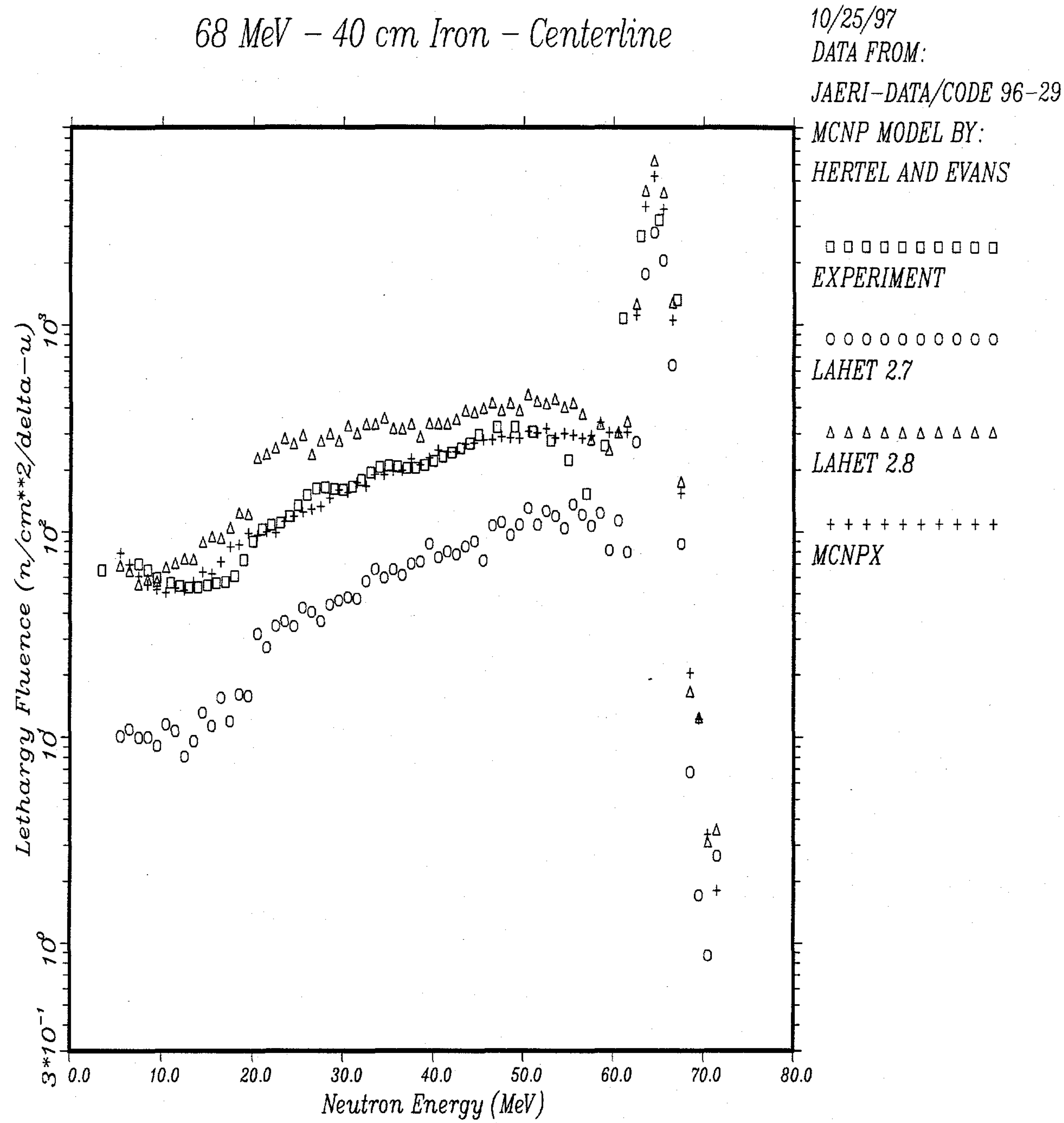

Fig. 1. Comparison of LAHET 2.7, LAHET 2.8 and MCNPX with experimental results in the JAERI experiment. The transmitted neutron fluence is measured and calculated immediately adjacent to the downstream side of the iron transmission target directly on the beam centerline.

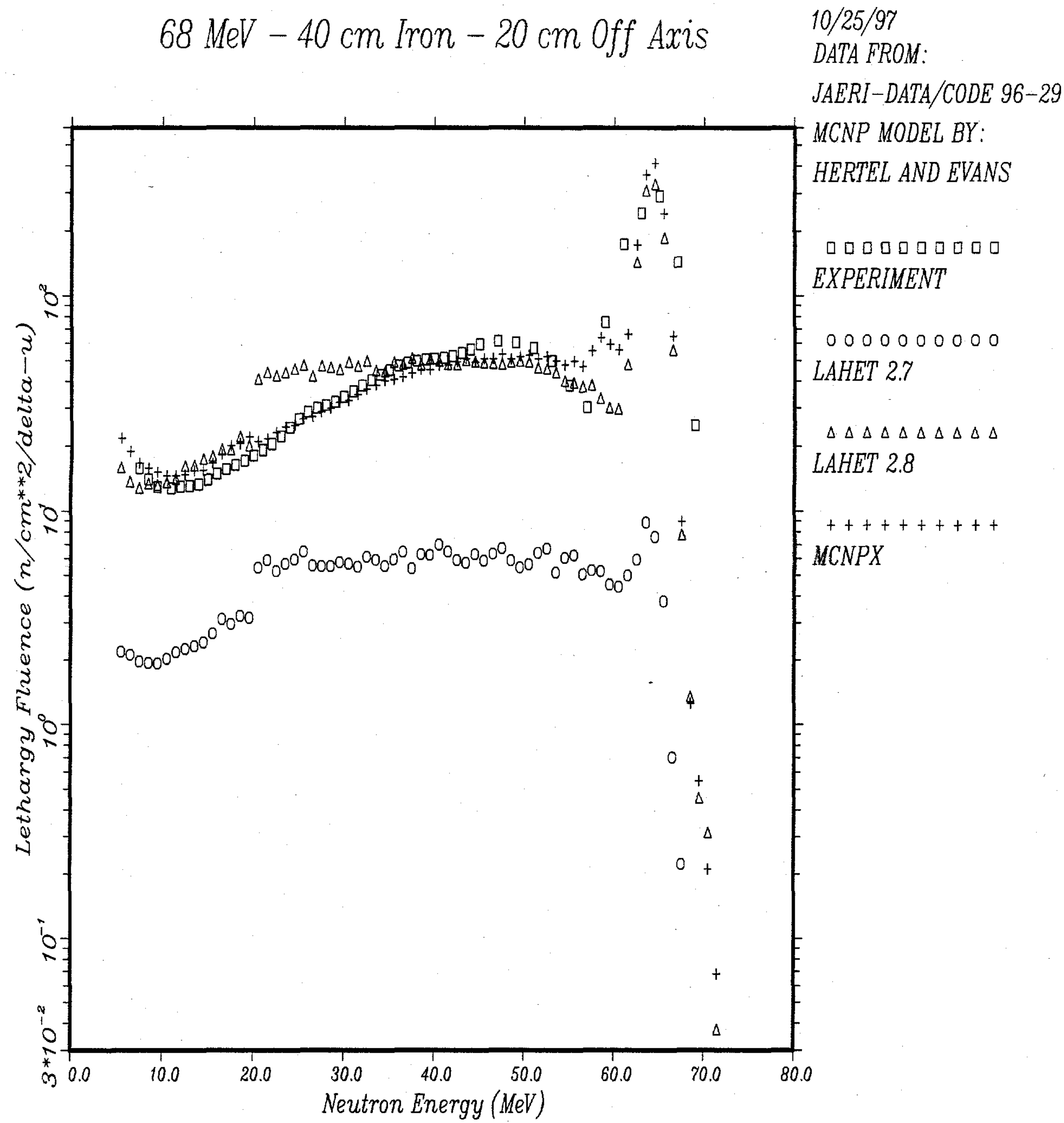

Fig. 2. Comparison of LAHET 2.7, LAHET 2.8 and MCNPX with experimental results in the JAERI experiment. The transmitted neutron fluence is measured and calculated immediately adjacent to the down-stream side of the iron transmission target at a position 20 cm away from the beam centerline.

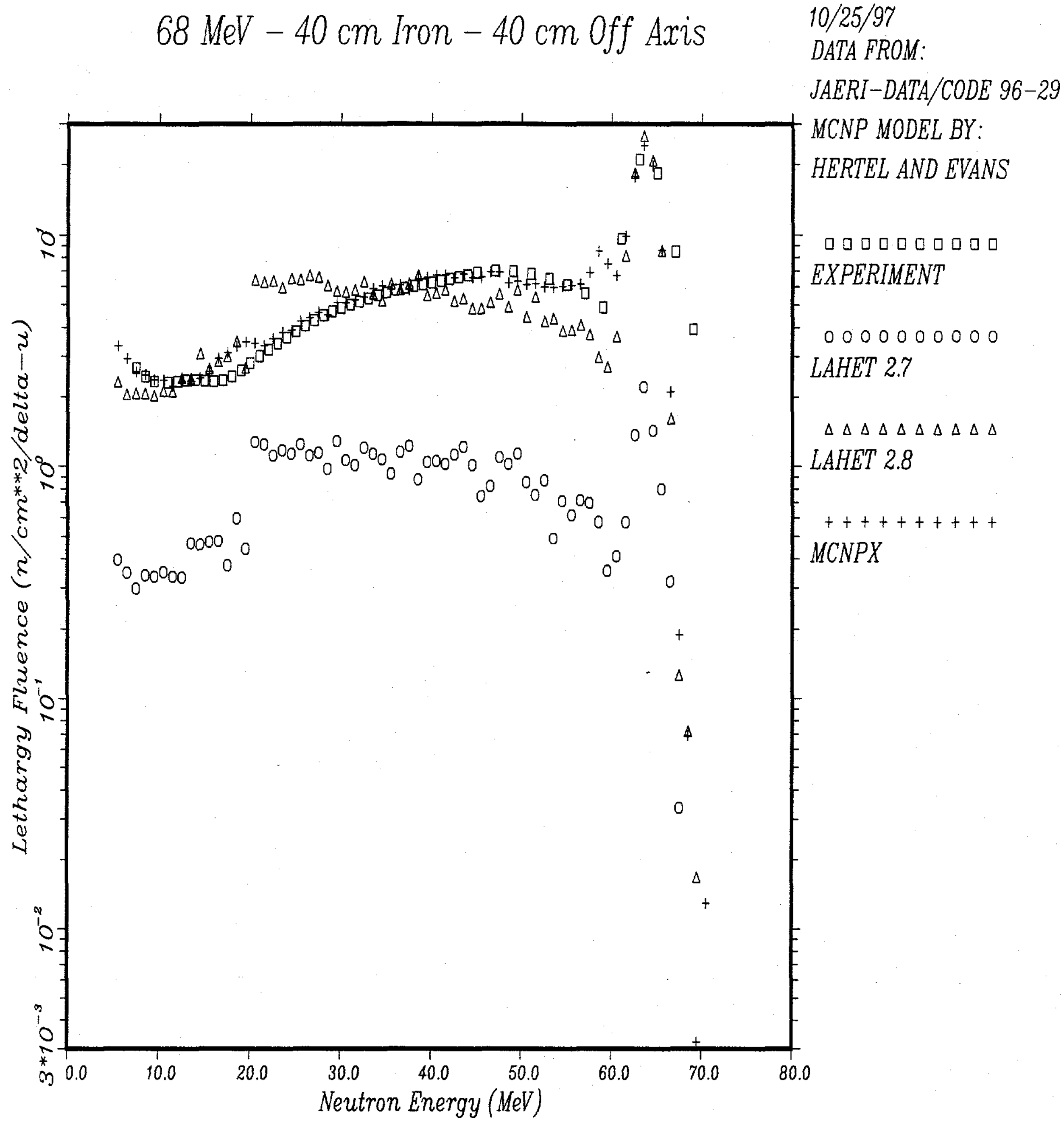

Fig. 3. Comparison of LAHET 2.7, LAHET 2.8 and MCNPX with experimental results in the JAERI experiment. The transmitted neutron fluence is measured and calculated immediately adjacent to the down-stream side of the iron transmission target at a position 40 cm away from the beam centerline.