r

6118 SEC4116 -- 1

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

LA-UR--85-1166

DE85 010794

TITLE: NUCLEAR DATA FOR MCNP

AUTHOR(S): Robert C. Little, X-6 Robert E. Seamon, X-6

SUBMITTED TO: Joint Los Alamos/CEA Meeting on Monte Carlo Methods, Cadarache, France, April 1985.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or asefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By accordance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royally-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the suspices of the U.S. Department of Energy



OS Alamos National Laboratory Los Alamos National Laboratory Los Alamos, New Mexico 87545

MAY 0 8 1995

NUCLEAR DATA FOR MCNP

۰.

Robert C. Little and Robert E. Seamon Radiation Transport Group Los Alamos National Laboratory Los Alamos, New Mexico 87545

The sources of neutron and photon transport data are described as well as the processing of the evaluated data sets into continuous-energy and multigroup cross-section sets. The procedures for checking and validating the processed data are discussed. The question of why so many data sets are available is addressed by indicating the differences between data sets as well as their relative strengths and weaknesses. Suggestions are made to help the MCNP user in selecting appropriate cross-section sets.

NUCLEAR DATA FOR MCNP

INTRODUCTION

In running transport problems with the Monte Carlo code MCNP, it is important to have information about what happens to the neutrons and photons when they collide with atoms of the materials through which they pass. This information is contained in the cross-section sets which contain representations of the physics of the interactions. For each constituent element or nuclide in a problem there is a set of numbers detailing through which processes the interactions might take place, and at which angles and with what energies the scattered particles are likely to emerge. In the case that photons are produced by the incident neutrons, you need information about the energy and angle at which the photons are produced as well as information about the scattered neutrons.

One thing is certain. It is the cross section data through which the differences between hydrogen and unanium are introduced into your transport calculations. The reason you specify material densities so carefully - the reason it matters how you specify those densities - is manifest in the macroscopic and microscopic cross sections used in the various regions of your problem. Careful geometry specifications are without much meaning if the physics going on inside the materials in the various regions of the geometry is incorrect. The cross sections contain the physics and that is why so much effort has gone into providing cross sections - ever since the beginning of Monte Carlo calculations at Los Alamos.

Connect data and connect physics are the most essential components of a successful transport code. Sloppiness with cross sections cannot be tolerated. It is important to understand what is going on with the cross sections and to understand the strengths and weaknesses of various cross-section sets. The purpose of this paper is to explain why there are so many cross-section files, to explain how they were created and checked, and to suggest a few matters for consideration when cross-section sets are chosen.

CLASSES OF DATA

There are three modes in which MCNP can be run; MODFO (reutron only problem), MODE1 (coupled neutron-photon problem), and MODE2 (photon only problem). In a MODE2 problem one has a neutron source with neutron transport; in a MODE2 problem one has a photon source with photon transport; in a MODE1 problem one has a neutron source with neutron transport and a neutron-induced photon source with photon transport. In order to run such problems, we need three basic kinds of data;

- 1) data describing the interactions of neutrons with nuclei,
- data describing the production of photons when neutrons interiet with nuclei, and

data describing now photons interact with nuclei.

The neutron interaction and photon production cross sections - the "neutron" files - are kept separate from the photon interaction files - the "photon" files. The "neutron" files are recuired for MODEO and MODE1 problems; the "photon" files are required for MODE1 and MODE2 problems. The separation of the "neutron" and the "photon" files has good reasoning behind it. Neutrons interact differently with different isotopes of the same nuclear species. and photon production by neutrons depends on the level structure of each particular isotope; the interaction of neutrons with a nucleus depende on the atomic number 2 and the mass number A of that nucleus. On the other hand, the interaction of photons with matter is really an atomic process: the interaction is with the electrons surrounding the nucleus and depends, therefore, only on the atomic mumber Z. It would be inefficient to carry the photon interaction cross sections in the same file with the neutron cross sections, bucause of the repetition of the same photon interaction information for various isotopes of the same element. The "neutron" data files which depend on Z and A are kept separate from the "photon" files which depend only on Z.

On the basis of the foregoing discussions, it would appear that the physics package should be contained in just two files - the "neutron" file and the "photon" file. There are, however, five classes of nuclear data tables which exist for MCNP:

- 1) continuous-energy neutron-interaction data (Class C),
- discrete-reaction neutron-interaction data (Class D),
- 3) photon-interaction data (Class P),
- 4) neutron dosimetry cross sections (Class Y), and
- 5) neutron $S(\alpha, f)$ thermal data (Class T).

In MCDE0 and MODE1 problems one continuous-energy or discrete-reaction neutron-interaction table is required for each isolope or element in the problem. Likewise, one photon-interaction table is required for each element in a MODE1 or MODE2 problem. Cross sections from dosimetry tables may be used as response functions with the FM card to determine reaction rates. Thermal $\mathcal{L}(\alpha,\beta)$ tables may be appropriate if the neutrons are transported at sufficiently low energies.

Each nuclear data table contained on any one of the five classes of data files is identified by a tennohymacter name, called the ZAID. The general form of a ZAID is UZAAA.nnX, where

22 is the atomic number, AAA is the mass number, nn is the data set identifier, and X indicates one of the five classes of data enumerated above.

SOURCES OF THE NUCLEAR DATA

To understand why there are multiple cross-section sets reallable, as represented by the evaluation identifier "nn" in the ZAID, it might be well to understand where the cross-section tables come from. Each table is generated from an evaluated data set. An evaluated set of cross sections is produced by analyzing experimentally measured cross sections and combining that data with the predictions of nuclear model calculations in an attempt to extract the most accurate cross section information. In an evaluated data set no ambiguity is allowed; for better or for worse, a decision has been reached on what the cross section for each reaction should be and what the secondary energy and angular distributions should be. If results from data testing indicate that serious discrepancies are caused by the use of a particular cross section evaluation, or if new and significant experimental results become available which are in serious disagreement with the evaluated data set, that set must be re-evaluated.

The preparation of evaluated cross-section sets is a real discipline in itself which has developed since the early 1960s. In America, workers in the thermal and fast reactor programs, the controlled thermonuclear reactor program, and the defense community joined forces to create the national system FNDF/B (Evaluated Nuclear Data File/B).

The differences between evaluated sets for the same isotope can be remarkable. The character of an evaluation depends on its age and on the style (techniques and attitudes) of the evaluator. Clearly, evaluations prepared in 1985 have the benefit of more and better experimental data than these prepared in 1960. It is the ENDF/B evaluations which seem to have gained worldwide acceptance because of the careful attention to details in every energy regime and the thorough testing and critical peer review they receive before release.

Users of MCNP are provided with the option of using "neutron" creas sections from a wide variety of sources, even for the same isotope. In recent years, the primary source of evaluated neutron-interaction and photon-production data for MCNP has been the ENDF/B system. Evaluated neutron-interaction tables have also been extracted from two other sources: the Lawrence Livermore National Laboratory's Evaluated Nuclear Data Library (FNDL) and evaluations from the Los Alamos Applied Nuclear Science Group (see, for example, Refs. 3-5). Older evaluations accessible to MCNP users gone from early versions of ENDF/B and ENDL, the Los Alamos Master Data File, and the Atomic Weapons Research Establishment at Aldermaston, England.

CONTINUOUS-ENERGY "NEUTRON" CROSS SECTIONS - CLASS C DATA

Evaluated data cannot be accessed directly by MCNP; available in various formats, it must first be processed into a single format recognized by MCNP. There is a separate format for each class of data. In the case of the "acutron" files, that format is the ACE (A Compact ENDF) format. The very complex processing codes used, for this purpose include NJOY for evaluated data in ENDF format and MCPOINT for ENDL data. Not all cross sections in ACE format were produced using these codes; they have been produced over a period of more than ten years by several people usin; various processing codes.

At Los Alamos we have available about 800 different "neutron" cross-section sets for 93 isotopes or materials. On the average there are nine different cross-section set possibilities for each combination of Z and A for which there are cross sections. The availability of several evaluation sources is not sufficient to explain why there are so many different sets for the same element or isotope. There can be several data sets produced from even one evaluation because of the linearization and thinning tolerances as well as the resonance reconstruction tolerances. There is also the matter of temperature broadening. This multiplicity exists only in the "neutron" files.

"Neutron" cross section files are complete in the sense that cross sections, angular distributions, and secondary energy distributions in one form or another are available; these COMPLETE sets are required for any material through which it is intended to transport neutrons in MODEO or MODE1 problems. The cross sections for producing photons along with the energy and angular distributions of the induced photons are also carried on the "neutron" files; not all "neutron" data sets include photon production data, however.

Cross sections for all reactions given in the evaluated data are specified. For a particular table, the cross sections for each reaction are given on one energy grid. This energy grid is sufficiently dense that linear-linear interpolation between points reproduces the evaluated cross sections within a specified tolerance that is generally one percent or less. All cross section tabulations given in the evaluated data with semi-log or log-log interpolation schemes have been linearized. Depending primarily on the number of resolved resonances for each isotope and the resonance reconstruction tolerance (generally 1/2% or better), the resulting energy grid may contain as few as 250 points (e.g., H-1) or as many as 32,500 points (e.g., Au-197). Other information, including the local absorption cross section, the total photon-production cross section, and the average heating number (for energy deposition calculations), is also tabulated on the same energy grid.

Much more than cross sections are included on the "neutron" files. Anrular distributions of scattered neutrons are included in the neutron-interaction tables for all non-absorption reactions. The distributions are given in the center-of-mass system for elastic scattering and discrete-level scattering, and in the laboratory system for all other inelastic reactions. Angular distributions are given on a reaction-dependent grid of incident neutron energies.

The sampled angle of scattering uniquely determines the secondary energy for clastic scattering and discrete-level inclastic scattering. For other inclastic reactions, energy distributions of the scattered neutrons and provided in the neutron-interaction tables. As with angular distributions, the energy distributions are given on a reaction-dependent grid of incident neutron energy.

When evaluations contain data about secondary photon production, that information appears in the MCNP neutron-interaction tables. Recently-processed data sets contain photon-production cross sections, photon angular distributions, and photon energy distributions for each reaction that produces secondary photons. The information is given in a manner similar to that described in the last few paragraphs for neutron cross sections and secondary neutron distributions. This expanded ACE format is described in Ref. 9.

Other miscellaneous information on the neutron-interaction tables includes the atomic weight ratio of the target nucleus, the Q values of each reaction, and nubar (the average number of neutrons per fission) data for fissionable isotopes. There are approximations that must be made when processsing an evaluated data set into ACE format. Cross sections are reproduced only within a certain tolerance; the tolerance is generally very small; to decrease it further would result in excessively large data tables. Evaluated angular distributions for secondary neutrons and photons are approximated on MCNP data tables by 32 equally-probable cosine bins. This approximation is clearly necessary when contrasted to the alternative that might involve sampling from a 20th-order Legendre polynomial distribution. Secondary neutron energy distributions given in tabular form by evaluators are sometimes approximated on MCNP data tables by 32 equally probable energy bins. Older "neutron" tables include a 30 x 20 matrix approximation of the secondary photon energy spectra.

It is the intent of those who prepare the ACE-format libraries to remove as little detail as possible from the basic evaluation. These "original" libraries, the first libraries produced in the processing of the date, are the libraries which in ACE format most closely represent the intent of the evaluators.

The 'original" files can be very long, indeed. Frequently users had trouble getting the "original" files from the common file system and even more trouble in fitting them into their MCNP problems. Therefore, a shortened or "thinned" set of cross sections in ACE format was prepared for the same ENDF/P materials. The PENDF files were thinned in such a way as to preserve the flat-weighted integral of the total cross section to within 0.5. Further reductions in length were effected by reducing the number of neutron energies at which the angular distributions are tabulated.

Since in the preparation of the "original" cross-section files the intention was to reproduce the evaluated data as closely as possible, a user has the right to ask what has been sacrificed by reducing the number of energies drastically in the "thinned" sets. It is almost totally from the resonance region that the energies have been removed. Hence, it is necessary only to worry about the total, elastic, fission, and radiative capture cross sections. If you plot the "original" and "thinned" cross sections on any sort of normal energy scale, it is difficult if not impossible to see any differences between the two curves.

When you plot the "original" and "thinned" cross sections on vastly expanded energy scales, you can see that some of the thin, narrow resonances have been smoothed over or even eliminated in the "thinned" cross sections. The elimination of resonances and the apparent shifting of the resonance energy, brought about by a change in the maximum value at a resonance, are not the only effects of thinning, however. When the plots are blown up, we see that the resonances which remain are effectively broadened because the minime of the curves are not so well defined. This broadening of resonances and changes in the cross-section values make themselves manifest in other ways as well. For example, multigroup cross sections are larger when calculated from the "thinned" set rather than from the "original" set. Multigroup numbers confirm what we first stated: the "original" and "thinned" cross-section sets differ essentially in the resonance regions. Detail has, of necessity, been sacrificed in order to hold down the size of the cross-section files. For problems in which exact detail in the resonance region is essential, it is clearly necessary to use the "original" cross sections.

The faithful preservation of the data has the advantage that the same Monte Carlo libraries can be used with confidence for general applications throughout the Laboratory. It suffers from the disadvantage that the crosssection sets as stored are much larger than necessary for some applications. Of course, once the cross sections have been read into MCNP, the code knows enough to "expunge" those data which are not needed. This can be effected through use of the energy cut-off cards.

DISCRETE REACTION "NEUTRON" CROSS SECTIONS - CLASS D DATA

In reproducing the evaluated nuclear data using one energy grid for all reactions and a sufficiently dense energy mesh such that all reactions are reproduced to within 0.1%, you can end up with some very large cross-section files. That is, of course, the reason we introduced the "thinned" crosssection sets. But even if you use "thinned" cross sections, the crosssection storage requirements for an MCNP problem can be quite large - large enough that the clock time for execution is remarkably increased when you are running in a time-sharing environment. Something had to be done to shrink the size of these enormous files so that problems could be run easily during the day for purposes of dobugging. These concerns led to the introduction of the discrete-reaction cross section files. The pointwise reaction cross sections have been averaged over 262 energy groups using a flat weight function. This has effected a shrinkage in total length of individual cross-section files by as much as a factor of 7. These discrete cross-section libraries are NOT multigroup libraries in the sense of scattering matrices which one could feed into the multigroup Monte Carlo code MCMG. The cross sections are given as histograms rather than as continuous curves; the remaining data (angular distributions, energy distributions, nubar, etc.) are identical in discrete-reaction and continuousenergy tables. The same comment holds for the "original" continuous-energy and the "thinned" continuous-energy cross sections. The secondary angular and energy distributions are essentially the same. Occasionally an angular aistribution is thinned out. The differences between the full continuous energy, the thinned continuous energy, and the discrete reaction crose sections are in the cross sections themselves - the bulkiest part of the files.

Discrete-reaction tables are provided primarily as a method of shrinking the amount of data storage required in order to enhance the ability to run MCNP on small machines or in a time-sharing environment. The tables are also useful for preliminary scoping studies. They are not, however, recommended as a substitute for the continuous-energy tables when performing final design calculations, particularly for problems involving transport through the resonance region.

MULTIGROUP REPRESENTATIONS

Calculations in MODEO, MODE1. or MODE2 can also be carried out using true multigroup cross section data with the multigroup variant of MCNP called MCMG. At Los Alamos we have available continuous-energy and multigroup cross sections derived from the same source of evaluated data using the NJOY processing code. We anticipate that multigroup cross section sets will become a sixth class of MCNP data (Class M) when the MCMG capability becomes a standard feature in MCNP.

PHOTON INTERACTION CROSS SECTIONS - CLASS P DATA

The Class P cross sections for the photon interaction data are stored on the library "" "B. There is only one evaluation for each value of Z; i.e., the AIDs is ZZ000.01P. The reason for the simplicity of the situaform of tion with regard to photons is the fact that the photon interaction cross sections have been so well understood theoretically for some time. The "photon" cross sections used up through the time of MCNP Version 2D came from the work of Storm and Israel' ^r published in 1970. This work was supplemented above 15 MeV with cross sections from the ENDF/B libraries. Now with MCNP Version 3 we are using all of the ENDF/B information provided on the library DLC-7 E^{13} distributed by the Radiation Shielding Information Center with the exception of data for Z=84, 85, 87, 88, 89, and 93 which still must come from Storm and Israel because they do not exist on DLC_4-7E . The fluorescence data are taken from work by Cashwell and Everett. Tt should be noted that the photon library MCPLIB based on DLC-7E does not differ that much from the old MCPLIB based on Storm and Israel.

Cross sections as a function of energy are given on the "photon" tables for coherent scattering, incoherent scattering, pair production, and the photoelectric effect. Energy grids are tailored specifically for each element and contain about 40-60 points. Log-log interpolation is employed to determine cross sections between adjacent energies. Heating numbers are tabulated on the same energy grid as the cross sections.

The determination of directions and energies of scattered photons requires information different from the sets of angular and energy distributions found on neutron-interaction tables. Angular distributions of secondary photons are introduced through form factors for coherent scattering and scattering functions for incoherent scattering. Form factors and scattering functions are tabulated as a function of momentum transfer on the photoninteraction tables. The energy of an incoherently scattered photon is calculated from the sampled scattering angle. Values of the integrated coherent form factor are tabulated on the photon-interaction tables for use in point detector routines.

Very few approximations are made in the various processing codes used to transfer photon data from ENDF into the format of MCNP photon-interaction data. Cross sections are reproduced exactly as given. Form factors and scattering functions are reproduced as given; however, the momentum-transfer grid on which they are tabulated may be different from that of the original evaluation. Heating numbers are calculated from the evaluated data. Fluorescence data are not provided in ENDF; therefore, the data for MCNP are extracted from a variety of sources as described in Ref. 14.

In MODE1 and MCDE2 problems, the photon cross sections are taken by default from MCPLIB, because there is only one "photon" library. There is no need to worry about specifying which photon interaction cross sections to use since the best available numbers are right there on MCPLIB.

DOSIMETRY CROSS SECTIONS - CLASS Y DATA

Dosimetry cross sections, the Class Y cross sections, are useful in tallying when you wish to calculate reaction rates by multiplying an energy-dependent fluence by the appropriate cross section. The reactions of interest are specified on the FM card; they are generally chosen from among those available on the Class C cross-section libraries used for the transport calculations. One is not limited to this very large set of reactions, however. There are cross sections for additional reactions on assorted isotopes available on the dosimetry cross-section libraries. These dosimetry cross sections are NOT full cross-section sets in ACE format with energy and angular distributions. Most likely the list of reactions is quite incomplete; frequently, there is only one reaction given for a particular isotope. The dosimetry cross sections cannot be used in transport calculations, but they are perfect for tallying.

Data contained on dosimetry tables are simply energy, cross-section pairs for one or more reactions. The energy grids for all reactions are independent of each other. Interpolation between adjacent energy points may be specified as histogram, linear-linear, linear-log, log-linear, or log-log. With the exception of the tolerance involved in any reconstruction of pointwise cross sections from resonance parameters, evaluated dosimetry cross sections are reproduced on the MCNP data tables without approximation.

NEUTRON THERMAL S(a, B) CROSS SECTIONS - CLASS T DATA

Thermal $S(\alpha, \beta)$ tables are never required. They may be used in MODEO or MODE1 problems, and should be used in such problems involving neutron thermalization. Thermal tables have ZAIDs of the form XXXXXX.nnT where XXXXXX is a mnemonic character string. The data on these tables encompass that required for a complete representation of thermal neutron scattering by molecules and crystalline solids.

The source of $S(\alpha,\beta)$ data is a special set of ENDF tapes.¹⁶ The THERMR and ACER modules of the NJOY system have been used to process the evaluated thermal data into a format appropriate for MCNP.

Data contained on the current thermal tables are for neutron energies less than 4 eV. Cross sections are tabulated on table-dependent energy grids; inelastic scattering cross sections are always given; elastic scattering cross sections are sometimes given. Correlated energy-angle distributions are provided for inelastically-scattered neutrons. A set of equally-probable final energies is tabulated for each of several initial energies. Furthermore, a set of equally-probable cosines or cosine bins is tabulated

.

for each combination of initial and final energy. Elastic scattering data may be derived from either a coherent or incoherent approximation. In the incoherent case, equally-probable cosines or cosine bins are tabulated for each of several incident energies. In the coherent case, scattering cosines are determined from a set of Bragg energies derived from the lattice parameters. During processing, approximations to the evaluated data are made when constructing equally-probable energy and cosine distributions.

PROMPT AND TOTAL NUBAR

For several fissionable isotopes the MCNP user has available the choice between prompt and total nubar, where nubar is the average number of neutrons per fission. Generally, the total fission nubar is desired for reactor-type or steady-state problems where the effect of delayed neutrons may be important. In problems where the neutron lifetime is so short that a steady-state condition is not reached, then the prompt nubar is appropriate. Not all evaluations for fissionable isotopes have been provided with both prompt and total nubar, and for some evaluations only the prompt nubar is given. For the most important fissionable isotopes in ENDF/B, both prompt and total nubar values are given. This matter should be given consideration when you are setting up MCNP problems.

VALIDATION OF CROSS SECTIONS

We are proud of the extensive nuclear data libraries which are available to MCNP users. Why are we confident that the intentions of the data evaluators are being faithfully represented? We have invested a tremendous effort in validating these data files. There are two types of data validation: integral data checking and differential data checking.

In Table I there is an outline of the areas in which MCNP and its associated data bases have been used successfully in calculations. References detailing much of these areas are given in Ref. 17; there are many other reports available in which calculations with MCNP are compared to experiments. In Ref. 18 calculations of the Army Pulsed Reactor Division measurements, the Oak Ridge National Laboratory "broomstick" measurements, and the Lawrence Livermore National Laboratory pulsed sphere experiments carried out with the view to renormalizing the air transport cross sections are described. Several other sets of pulsed sphere calculations are described in Refs. 19-25. The bulk shielding calculations done for the Antares Laser Fusion Facility were carried out using the MCNP Monte Carlo code.

An extensive series of benchmark calculations on thermal critical assemblies has been carried out using MCNP with ENDF/B-IV data. The calculations were undertaken to document the thermal scattering model and the improvements in the treatment of the $S(\alpha, \beta)$ scattering law data as implemented in MCNP. The results are given in detail in eleven tables in Ref. 26.

Infinite lattice benchmark calculations using MCNP with ENDF/B-IV data for light-water-moderated uranium metal fueled assemblies, for the light-water-moderated uranium oxide fueled assemblies, and for a heavy-water-moderated

uranium metal fueled assembly have been performed. Infinitely long hexagonal cells with reflective boundary conditions were used; the results were reported in detail in Ref. 27.

Extensive neutronics calculatons for magnetic fusion reactor designs such as the Elmo Bumpy Torus (EBT), Linus, Reversed Field Pinch Reactor and Fast-Liner Reactor concepts have also been carried cut using MCNP.

The success of the calculations mentioned above plus many others stands as a commentary on the MCNP code and the data bases associated therewith. If in MCNP calculations we handle the nuclear data as the evaluators intended, the successful calculations would indicate that the evaluators have done their jobs well. It is true that disagreement between calculated and experimental numbers has been known to point to flaws in the ACE-formatted cross sections; that's why we calculate these experiments. But more frequently the lack of agreement between calculation and experiment can be traced back to problems in the evaluations themselves; in this way we find ourselves an integral part of the nuclear data evaluation cycle. Our criticisms of evaluations based on the results of MCNP calculations will be meaningless if the data are not handled in the code as the evaluators intended. Checking the pointwise data files themselves as processed into ACE format by the NJO* code is what we refer to as "differential" data checking. We look at the files directly and calculate quantities therefrom for comparison with the same quantities calculated from the original evaluation. The bulk of the "differential" checking effort is spent in examining the bulkiest part of the ACE libraries - the energy dependent reaction cross sections. Sets of multigroup cross sections are calculated from the original ENDF/B cross sections and from the cross sections in ACE format using the same weight function. One does not expect the corresponding multigroup numbers to be identical due to the effects of linearization of the original data and due to thinning, but it is amazing the discrepancies in ACE-formatted data that have been pointed out. You can be sure that anomalously poor comparisons point to some sort of problem in the data translation.

There are other tests and many plots made for comparison from both the ACE and the original evaluated data. The most disconcerting aspect of this checking effort is that automation thereof is only part of the battle. Eternal vigilance is the price of accuracy.

CHOOSING YOUR CRUSS SECTIONS

The matter of how to select neutron-interaction tables appropriate for your calculations will now be discussed. Multiple tables for the same is tope are differentiated by the "nn" portion of the ZAID. The easiest choic for the user, although by no means the recommended one, is not to enter the "nn" at all. This will force MCNP to select the default tables based simply on those tables that are found first in the cross-section directory file XSDIR. Including a DRXS card in the input file will force MCNP to choose the default discrete-reaction tables.

4

Why not just use the default cross sections? What's wrong with them? NCTHING is WRONG with them. They are frequently the very best cross sections we have to offer. Careful users will want to think about which

"neutron" cross-section tables to choose. There is, unfortunately, no strict formula for guidance in choosing the tables. The best that can be offered is a series of guidelines and observations: 1) Users should be conscious of the differences between the "original", "thinned", and discrete cross sections. The evaluation source is the same; the "original" ACEformatted cross sections reproduce the evaluated data most faithfully. "Thinned" cross sections have been processed with less rigid tolerances. Discrete-reaction cross sections are given as histograms. For high-energy problems the thinned and discrete-reaction data are probably not bad approximations. Conversely, it is essential to use the most detailed continuous-energy set available for problems influenced strongly by transport. through the resonance region; 2) Users should be conscious of the dif . ferences in evaluators' philosophies. The evaluations from the Physical Data Group at Livermore (ENDL) manifest a philosophy of representing the experimental data with the fewest possible raints. Evaluations from the Applied Nuclear Science Group at Los Alamos are frequently the most complex because they are the most thorough; 3) Check the temperature at which various data tables have been processed. Do not use a set that is Dopplerbroadened to 12 million degrees K for a room-temperature calculation; 4) Check the sensitivity of your results to various sets of nuclear data. Try, for example, a calculation with ENDF/B cross sections, and then repeat the calculation with ENDL cross sections. If the results of a problem are extremely sensitive to the choice of nuclear data, it is advisable to find out why. Much insight into your calculation can be gained from understanding these differences; 5) For a MODE1 problem, be careful to choose cross section tables with which photon production data are available. If possible, use the more recent sets that have been processed with expanded photon production; 6) As a general rule, use the best cross section data you can afford. It is understood that the latest evaluations tend to be more complex and, therefore, require more memory and longer execution times. If you are limited by available memory, try to use "thinned" data tables for the minor isotopes in your calculation. Discrete reaction tables might be used for a parameter study, followed by a calculation with the full continuous energy data tables for confirmation.

The additional time required to choose appropriate neutron-interaction data tables rather than simply to accept the defaults will be repaid in the understanding of your calculation which is gained thereby.

CONCLUSION

The glory of continuous-energy MCNP is that one can model the geometry and particle transport in difficult problems nearly exactly. The possibilities of representing complicated geometries in MCNP are limited only by the dedication of the user. That dedication pays off, because in reproducing the intentions of cross-section evaluators, MCNP stands second to none in the faithful utilization of even the most sophisticated ENDF/B evaluations.

÷

REFERENCES

- R. Kinsey, "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," Brockhaven National Laboratory report BNL-NCS-50496 (ENDF-102) 2nd Edition (October 1979).
- R.J. Howerton, D.E. Cullen, R.C. Haight, M.H. MacGregor, S.T. Perkins, and E.F. Plechaty, "The LLL Evaluated Nuclear Data Library (ENDL): Evaluation Techniques, Reaction Index, and Descriptions of Individual Evaluations," Lawrence Livermore National Laboratory report UCRL-50400, Vol. 15, Part A (September 1975).
- E.D. Arthur and P.G. Young, "Evaluated Neutron-Induced Cross Sections for 54,56Fe to 40 MeV," Los Alamos Scientific Laboratory report LA-862(-MS (ENDF-304) (December 1980).
- D.G.Foster, Jr. and E.D.Arthur, Average Neutronic Properties of "Prompt" Fission Products," Los Alamos National Laboratory report LA-9168-MS (February 1982).
- E.D. Arthur, P.G. Young, A.B. Smith, and C.A. Philis, "New Tungsten Isotope Evaluations for Neutron Energies Between 0.1 and 20 MeV," Trans. Am. Nucl. Soc. 39, 793 (1981).
- M.W. Asprey, R.B. Lazarus, and R.E. Seamon, "EVXS: A Code to Generate Multigroup Cross Sections from the Los Alamos Master Data File," Los Alamos Scientific Laboratory report LA-4855 (December 1973).
- R.E. MacFarlanc, D.W. Muir, and R.M. Boicourt, "The NJOY Nuclear Data Processing System, Volume I: User's Manual," Los Alamos National Laboratory manual LA-9303-M, Vol. I (ENDF-324) (May 1982).

R.E. MacFarlane, D.W. Muir, and R.M. Poicourt, "The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THEEMR Modules," Los Alamos National Laboratory manual LA-9303-M, Vol. 11 (ENDF-324) (May 1982).

- R.J. Howerton, R.E. Dye, P.C. Giles, J.R. Kimlinger, S.T. Perkins, and E.F. Plechaty, "Omega Documentation." Lawrence Livermore National Laboratory report UCRL-50400, Vol. 25 (August 1983).
- R.C. Little and R.E. Seamon, "Neutron-Induced Photon Production in MCNP," Proceedings of the Sixth International Conference on Radiation Shielding, Tokyo, Japan, May 16-20, 1983, Vol. I, pp.151-160.
- D.G. Collins and W.M. Taylor, "MCMG-Update," Los Alamos National Laboratory internal memorandum to Croup X-6 (September 27, 1983).
- 11. R.C. Little, "Cross Sections for Version 3 of MCMG," Los Alamos National Laboratory internal memorandum X-6:RCL-85-9 to Distribution (January 8, 1985).

- 12. E. Storm and H.I. Israel, "Pnoton Cross Sections from 0.001 to 100 MeV for Elements 1 Through 100," Los Alamos Scientific Laboratory report LA-3753 (June 1967); ibid., "Photon Cross Sections from 1 keV to 100 MeV for Elements Z=1 to Z=100," Nuclear Data Tables A7, 565 (1970).
- 13. J.H. Hubbell, Wm.J. Veigele, E.A. Briggs, K.T. Brown, D.T. Cromer, and R.J. Howerton, "Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections," J. Phys. Chem. Ref. Data 4, 471 (1975); ibid., "Erratum: Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections," J. Phys. Chem. Ref. Data 6, 615 (1977).
- 14. C.J.Everett and E.D. Cashwell, "MCP Code Fluorescence-Routine Revision," Los Alamos Scientific Laboratory report LA-5240-MS (May 1973).
- 15. R.C. Little, "New Photon Library from ENDF Data," Los Alamos National Laboratory internal memorandum to W.L.Thompson (February 26, 1982).
- J.U. Koppel and D.H. Houston, "Reference Manual for ENDF Thermal Neutron Scattering Data," General Atomics report GA-8744, Revised (ENDF-269) (July 1978).

1

:

- W.L. Thompson and E.D. Cashwell, "The Status of Monte Carlo at Los Alamos," Paper I in Los Alamos Scientific Laboratory report LA-8353-MS (May 1980).
- G.P. Estes, R.C. Little, R.E. Seamon, and P.D. Soran, "Air Transport in Connection with the Hiroshima-Nagasaki Dose Reevaluation Effort," Los Alamos National 'aboratory report LA-9369-MS (July 1982).
- 19. G.P. Estes, "Pulsed Sphere Calculations with ENDF/B-V Cross Sections, (for transmittal to CSEWG)," Los Alamos Scientific Laboratory internal memorandum to R.E. MacFarlane (October 24, 1979).
- 20. G.P. Estes and R.E. Seamon, "Pulsed Sphere Calculations with ENDF/B-V Cross Sections (for transmittal to CSEWC)," Los Alamos Scientific Laboratory internal memorandum to P.G. Young and R.E. MacFarlane (May 9, 1980).
- 21. G.P. Estes and R.F. Seamon, "More Integral Testing of ENDF/B-V Data," Trans. Am. Nucl. Soc. 35, 460 (1980).
- 22. G.P. Estes, R.C. Little, R.E. Seamon, and P.G. Young, "Tools for Examining ENDF/B Data Prepared for Monte Carlo Calculations," Trans. Am. Nucl. Soc. 38, 568 (1981).
- 23. G.P. Estes, R.C. Little, R.E. Seamon, E.D. Arthur, and P.D. Soran, "Calculations Using New Tungsten Isotope Evaluations," Trans. Am. Nucl. Soc. 39, 794 (1981).
- 24. G.P. Estes, R.C. Little, and R.E. Seamon, "ENDF/R-V Data Testing for H, N, and O," Los Alamos National Laboratory memorandum to Robert W. Roussin, Chairman, CSEWG Shielding Data Testing and Applications Subcommittee (November 23, 1981).

- 25. G.P. Estes, "Preliminary Pulsed Sphere Calculations for Liquid Air," Los Alamos National Laboratory internal memorandum to Paul Whalen (January 14, 1981).
- 26. R.E. Prael, 'Summary of Thermal Reactor Benchmark Calculations Using MCNP with ENDF/B Version IV Data," page 30 in Los Alamos Scientific Laboratory progress report LA-8232-PR (February 1980).
- 27. R.E. Prael, "Infinite Lattice Benchmark Calculations Using MCNP with ENDF/B Version V Data," page 38 in Los Alamos Scientific Laboratory progress report LA-8232-PR (February 1980).
- C.G. Bathke, D.J. Dudziak, R.A. Krakowski, "ELMO Bumpy Torus Reactor and Power Plant - Conceptual Design Study," Los Alamos National Laboratory report LA-8882-MS (August 1981).
- 29. R.W. Miller and R.A. Krakowski, "Assessment of the Slowly-Imploding Liner (Linus) Fusion Reactor Concept," Los Alamos Scientific Laboratory report LA-UR-80-3071 (October 1980).
- R.L. Hagenson, R.A. Krakowski, and G.E. Cort, "The Reversed-Field Pinch Reactor (RFPR) Concept," Los Alamos Scientific Laboratory report LA-7973-MS (August 1979).
- 31. R.W. Moses, R.A. Krakowski, and R.L. Miller, "A Conceptual Design of the Fast-Liner Reactor (FLR) for Fusion Power," Los Alamos Scientific Laboratory report LA-7686-MS (February 1979).

TABLE I MCNP APPLICATIONS

Nuclear Safeguards Well logging Radiation shielding studies Radiation safety Physics experiments Energy deposition in materials Reactor design CTR neutronics Radiography Data verification Instrument design Radiation damage of material Material activation