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EVALUATED NUCLEAR DATA FILE ENDF/B-VI

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Abstract: For the past 25 years, the United States Department of Energy has sponsored a cooperative program among its laboratories, contractors and university research programs to produce an evaluated nuclear data library which would be application independent and universally accepted. The product of this cooperative activity is the ENDF/B evaluated nuclear data file. After approximately eight years of development, a new version of the data file, ENDF/B-VI has been released. The essential features of this evaluated data library are described in this paper.

(evaluated nuclear data, ENDF/B, nuclear reactions)

Introduction

In 1966, the United States Atomic Energy Commission, predecessor to the US Department of Energy, initiated a program to provide a nuclear data base which could be used in its research and development activities. This data base was intended to replace the many individual libraries then in use and provide a common reference point for evaluating proposals and research results. This data base was to be constructed from the results of nuclear data evaluation activities by contractors and coordinated through the Cross Section Evaluation Working Group (CSEWG) organized by the National Nuclear Data Center at BNL. The Evaluated Nuclear Data File data system which evolved in the intervening period consists of evaluated nuclear data in a format designed for computer processing along with the processing programs which can serve as a reference standard. The evaluated data added to the file are based on the best microscopic measurements and theoretical models available and validated against well tested benchmark experiments using the most advance calculational models available. The format and the cooperative approach to the production of an evaluated nuclear data library have served as models for similar activities throughout the world.

As a result of this coordinated effort, six versions of the ENDF/B data library have been completed. The most recent version, ENDF/B-V, was released in 1979 with an update in 1982. For the first time in its history, the distribution of significant parts of the ENDF/B data

library was restricted to users from the United States and AECL, Chalk River, Canada by the sponsoring agency. Requests for release of specific evaluations were treated on a case by case basis. This decision to restrict ENDF/B distribution by the sponsoring agency did not have much support within CSEWG and caused much displeasure among the world wide community which used ENDF/B data. While the restriction on information flow generally has a strong negative effect on base technology development, in this case there was one positive result, namely the development of strong independent evaluation projects outside the United States.

The primary sponsorship of CSEWG and the ENDF evaluation activity changed in the early 1980's from reactor development projects to basic research programs. This change in sponsorship had two important manifestations, namely a drastic reduction in funding and a committment to remove restrictions on the distribution of the next version of the ENDF/B data file. The reduction in resources has led to increased interest on the part of CSEWG in developing non-CSEWG contributions to its activities.

In 1989 and 1990, a new version of the ENDF/B library, ENDF/B-VI, was released. Many of the evaluations for neutron interactions with important nuclides have been revised, most completely reevaluated. Separate Activation and Dosimetry libraries are no longer available. For consistency, they are derived from the full evaluations. The remaining portions of ENDF/B-VI,

namely the decay data and the neutron fission product yields, will be completed and released this year. We also expect to have a small charged particle library for light mass materials available in the near future. CSEWG laboratories supplying evaluations are

ANL	Argonne National Laboratory, Illinois
ANL-West	Argonne National Laboratory, Idaho
BNL	Brookhaven National Laboratory
HEDL	Hanford Engineering Development Laboratory
INEL	Idaho Nuclear Engineering Laboratory
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
ORNL	Oak Ridge National Laboratory

Goals for ENDF/B-VI

The initial planning for ENDF/B-VI began in 1980 with a conference on evaluation methodology[1], held at Brookhaven National Laboratory in September of that year. This conference attracted international participation with the aim of assessing the current state of the art of nuclear data evaluation and discussing developments which would affect the next version of ENDF/B and other evaluated nuclear data libraries.

Two major goals were adopted at the earliest planning stages of the evaluation effort. These were **the production of a self-consistent set of evaluated neutron**

standard cross sections and improved data at energies important to fusion reactor design. In addition, CSEWG sought to improve the secondary energy balance in the important material evaluations, leading to an emphasis on isotopic evaluations in place of natural element evaluations where possible. It was recognized early in the evaluation cycle that the resonance region evaluations for the important fissile and fertile materials were out-of-date and in need of an intensive evaluation effort. However resources could not be identified immediately for the task. Only at a later stage were the resources found to accomplish this task using expertise from US and non-US evaluators.

It was recognized that the resources within CSEWG were insufficient to perform all the evaluations required. Work had to be deferred in some areas where we knew that significant improvements could be made. The most important of these areas were evaluations for fission product nuclides and for the trans-plutonium nuclides. Only limited improvements in these areas were made, in part by US evaluation efforts and in part by incorporating non-US evaluations in ENDF/B-VI. No separate evaluations of dosimetry and activation cross sections were made.

ENDF Formats

Traditionally, the ENDF data file format was the sole responsibility of the Methods and Formats Committee

of CSEWG. However, increased use of the ENDF format by evaluators around the world in the early eighties led to its de-facto adoption as the international standard for evaluated nuclear data. In recognition of this fact, CSEWG has actively sought to incorporate needs from a wider community in its format determination process. In 1984, the IAEA sponsored a meeting[2] to discuss the international community's requirements for ENDF format improvements and revisions. Several suggestions which were proposed at this meeting were included in the latest ENDF format specifications[3], ENDF-6.

In order to represent charged-particle reactions in the ENDF format, information identifying not only the target material but also the incident particle is required. Such information was added to "File 1" and the concept of a sublibrary was developed. In general, a sublibrary represented all evaluations with a common incident particle. Special cases of this concept included a neutron thermal scattering law sublibrary, a decay data sublibrary and a neutron fission product yield sublibrary. Unique identification of a library, its version and its format were also added to the "File 1" contents.

Major new resonance region formats were adopted to permit use of R-function and Generalized R-matrix representations. The Reich-Moore format was approved for use in structural material evaluations. A flag was added to signal whether the unresolved resonance region parameters should be used to calculate the cross section in that energy region, or only for self-shielding calculations.

A new file, "File 6", has been added to the format to permit a complete description of secondary particle energy-angle distributions. This new format is important at energies above a few MeV for fusion applications. All outgoing particle distributions can be described, including those for recoil nuclei. In addition to improved transport calculations from the correlated energy-angle distributions, kerma calculations can be done directly with information given in file 6.

Beginning with ENDF/B-IV, the ENDF/B library included uncertainties and covariance matrices. The formats for this information have been constantly improved and broadened to cover more data types. The covariance formats for resonance parameter representation were improved for ENDF-6 and new formats for secondary neutron angular and energy distributions and for isomer production cross sections added. Very late in the format development came a proposal to create a more general format, "File 30", which could be used to include covariance data resulting from model parameterization. While approved, this format has not yet been implemented in ENDF/B-VI.

Standards Evaluation

Considerable resources were devoted to the simultaneous evaluation of the standard neutron reaction cross sections[4]. Several heavy element reaction cross sections were included in this evaluation because of their close link to the standards via ratio measurements. Also included

in this activity were the thermal neutron cross sections for the important fissile and fertile nuclides. The evaluation process was a joint effort of ANL-West, LANL, ORNL and NIST under the auspices of the Standards subcommittee of CSEWG. Extensive non-overlapping experimental data bases were developed at LANL and ANL-West. LANL concentrated on R-matrix fits to the ^{6}Li and ^{10}B reactions, while ANL-West handled the remainder of the heavier standards plus some ^{6}Li and ^{10}B data with a generalized least squares simultaneous evaluation. The results from the two separate evaluations were merged at ORNL using both the data and covariance matrices in a comprehensive combination procedure.

The final results have been carefully reviewed by both CSEWG and the JEF Standards Committee. The results represent a considerable and perhaps definitive effort in this area. The major criticisms have been mainly due to a) the very small uncertainties which result from the analysis and b) the inconsistency in some of the results for ^{10}B, which probably result from the relatively poor experimental data base for that standard.

The cross sections for the neutron standard reactions resulting from this analysis were included in the ENDF/B-VI evaluations. However, representation of the covariance matrices can be best accomplished through use of the new generalized covariance format which has not yet been implemented. The cross sections for the thermal standards and for ^{238}U(n,γ) reaction were also incorporated in ENDF/B-VI. Results for the ^{239}Pu(n,f) cross

section were also used after slight scaling.

Structural Materials

Complete new evaluated data files for the major structural materials were prepared at ORNL. New evaluations were made for the separate isotopes of Cr, Fe, Ni, Cu and Pb. The resonance parameters for the major Fe and Ni isotopes represent a comprehensive fit to transmission, differential scattering, and capture measurements using the Reich-Moore model. In these cases, the resonance energy region was extended to significantly higher energies. Extensive precompound/compound nuclear model calculations were performed above the resonance region to provide particle and gamma-ray production cross sections, and correlated energy-angle distributions for secondary neutrons in the "File 6" format. Careful attention was paid to secondary energy balance. Complete cross section uncertainty files were provided for each evaluation. An evaluation for ^{55}Mn was completed at ORNL by a visiting scientist from JAERI and is included also in the JENDL-3 evaluated data file.

Evaluations for natural V, ^{59}Co, ^{89}Y, ^{93}Nb, natural In, ^{209}Bi and ^{115}In isomer production were done as a cooperative effort between ANL and LLNL. The high energy part of the evaluation included recent experimental results for total and elastic scattering data measured at ANL. Optical model calculations based on fitting this experimental data were used in calculating charged particle

production cross sections. Thermal data, resonance parameters and gamma-ray production cross sections were supplied by LLNL. Uncertainty files are included

Light Materials

The majority of the light material evaluations were the responsibility of LANL. R-matrix analysis for the standards materials, ^{1}H, ^{3}He, ^{6}Li, ^{10}B, ^{14}N and ^{16}O were included in the new evaluations. Charged particle production cross sections for ^{6}Li and ^{10}B were obtained from analysis of experimental data. Revised evaluations for ^{7}Li and ^{15}N were prepared as was a complete new evaluation for ^{11}B. The previous evaluation of ^{11}B had been done more than 20 years ago at AWRE and was badly out of date. No covariance files are supplied with these evaluations.

An extensive Monte-Carlo simulation to evaluate the (n,2n) reaction was included in a complete re-evaluation of ^{9}Be supplied by LLNL. In addition, a new evaluation of ^{19}F was performed at ORNL by a visiting scientist from P.R. China and included in ENDF/B-VI. A new evaluation for natural C was also supplied by ORNL. This evaluation extended up to 32 MeV and included all of the charged particle emission channels up to that energy. Covariance files were supplied for both C and ^{19}F.

Heavy Nuclides

The evaluation responsibility for the heavy nuclide evaluations for ^{235,238}U and ^{239,240}Pu were shared by LANL and ORNL. The data evaluation for energies above the unresolved resonance region was performed by LANL and is based on theoretical analysis of existing experimental data. The thermal and resonance region evaluations were the responsibility of ORNL. The evaluations for the standard and related cross sections were directly merged into the new evaluations. Complete evaluations for ^{241}Pu and ^{243}Am were performed at ORNL, for ^{237}Np at LANL and for ^{236}U at HEDL.

Significant new work for these nuclides included the reevaluation of the resonance parameters for ^{235,238}U and ^{239,241}Pu. Careful analysis of available high-quality experimental data was done using the latest resonance region fitting programs. The ^{238}U resolved resonance evaluation was done at Harwell and extended the resonance region to 10 keV. The unresolved resonance region evaluation was done at Karlsruhe. Included were 801 s-wave and 1112 p-wave resonances. The ^{235}U resonance region evaluation was performed at ORNL. The evaluation contains 3342 s-wave resonances in 10 energy regions up to 2.25 keV. The ^{239,241}Pu resonance evaluations were performed at ORNL by a visiting scientist from Caderache, France. These new evaluations extend the resolved resonance range up to 2 keV and 300 eV respectively, and are contained in both the ENDF/B-VI and JEF-2 data libraries, representing an example of significant data improvement resulting from international collaboration.

For the first time, complete evaluations performed outside the CSEWG organization have been included in a release of the ENDF data library. These are evaluations for ^{241}Am, ^{248}Bk and ^{248}Cf, provided by the Chinese Nuclear Data Center, Beijing.

Other Evaluations

Several fission product nuclide evaluations were modified at ORNL, primarily by updating the resonance parameters. Complete new evaluations for ^{151,153}Eu, ^{165}Ho and ^{197}Au were provided by LANL. The gold evaluation contained the recommended capture cross section from the standards analysis. Revised evaluations for ^{185,187}Re were provided by ORNL. The evaluations incorporated a new theoretical analysis of all reactions performed at LANL which took into account new capture measurements made at ORNL.

A significant improvement in the delayed fission neutron yields and spectra for all the important fissionable nuclides was made at LANL. The spectra were calculated from first principles using the latest decay data and neutron precursor yields and included in the ENDF/B-VI evaluations.

An updated decay data library has been prepared by INEL, LANL and HEDL. The starting point has been the ENSDF[5] data file supplemented by new data at INEL and theory at LANL. Final formatting and checking was done at HEDL. This data is being used in the evalua-

tion of fission product yields at LANL. These parts of ENDF/B-VI have not yet been released.

For the first time, charged particle and high energy evaluations have been included in ENDF/B-VI. The p-p and p-^{3}He evaluations were supplied by LANL. Evaluations of neutron and proton induced reactions on ^{56}Fe up to 1 GeV were supplied by BNL.

Validation Procedures

The new and revised evaluations included in ENDF/B-VI have undergone extensive review. Completed versions of evaluations were sent to BNL for final processing by the ENDF checking codes maintained by BNL. For the first time these codes had been used by the evaluating laboratories as part of the final file preparation. Kits were prepared including the checking code results, listings and plots of the evaluated data. These review kits contained overlays of cross sections from the new evaluations, ENDF/B-V and experimental data which appeared in the neutron data atlas[6] produced by NNDC. These kits were reviewed in detail at regular and special CSEWG meetings with the evaluators present in most cases. A document summarizing the new neutron evaluations contained in ENDF/B-VI is ready for publication[7].

Testing of this library against integral experiments has begun. This work has been delayed by lack of funding and delays in making the processing systems operational

at some of the data testing laboratories. The results currently available are encouraging. Thermal reactor data testing results have been obtained only for ^{235}U assemblies. ENDF/B-VI results are similar to ENDF/B-V except the trend of increasing eigenvalue as a function of epithermal leakage and epithermal fission fractions has significantly improved. In the fast reactor area, results show a slight improvement, although there are still areas of concern. For example, k_{eff} for larger assemblies such as BIG-10, ZPR-6/6A and ZPR-6/7 appear to be about 1% high, although there is greater consistency between ^{235}U and ^{239}Pu assemblies. The k_{eff} for Pu-fueled assemblies has increased and is close to 1.0. The ^{238}U capture to ^{235}U fission ratio and to ^{239}Pu fission ratio have improved. The dosimetry reaction evaluations do not perform as well as in ENDF/B-V, in particular, the ^{58}Fe and ^{59}Co (n,γ) reactions.

Future Plans

There are no plans for a complete new release of the ENDF/B data library at this time. CSEWG will continue to operate in a maintenance mode while awaiting the results of integral data testing, the revitalization of reactor development programs and the growth of other nuclear applications. We expect to release an upgrade to ENDF/B-VI which will contain corrections to known errors, additional uncertainty files and a few new evaluations in 1992 or 1993. We will make maximum use of the NEACRP/NEANDC sponsored cooperation among the

NEA countries on nuclear data evaluation and contribute where interest and resources permit. Where possible, we will make use of evaluations from other data files where they are better than the existing evaluation in ENDF/B.

Summary

A new version of the ENDF/B evaluated data library, ENDF/B-VI, has been completed and released for unrestricted distribution. It is available from the nuclear data centers at Brookhaven, Saclay, Vienna and Obninsk. Despite drastically reduced resources, significant improvements to the ENDF/B-V data library were made, in part due to increased international cooperation.

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