Proceedings of the Seminar on

NJOY–91 and THEMIS

for the Processing of Evaluated Nuclear Data Files

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FOREWORD

New versions of the EFF, ENDF/B, FENDL and JEF evaluated data files have been released in the last several years mainly for benchmarking purposes. All of them have adopted ENDF-6 formats for storing data. These formats are designed for storing not only data of neutral but also charged incident particles; they include new representations of data to allow more recent nuclear theory to be used in evaluations and improved treatment in applications.

NJOY has been adopted by many laboratories and projects for processing ENDF-6 format data files. Because of the new formats used in the evaluations, large parts of NJOY had to be rewritten. All modified or new software has to undergo thorough testing before it becomes reliable. The versions of NJOY and THEMIS presented at this seminar are the result of many severe tests in processing and the ensuing corrections and improvements. They contain additional modules which extend their capabilities.

The aim of the seminar was to bring together authors and users of the codes and evaluated data files for presenting the most recent developments of the codes, to discuss their performance, and to exchange know-how on the methods and recipes best suited for an efficient processing of the most recent evaluations.

This seminar has been suggested and encouraged by the OECD/NEA Data Bank Management Committee and the JEF Scientific Coordination Group.

NJOY-91 has been contributed to the NEA Data Bank computer program library through the Radiation Shielding Information Center, ORNL, Oak Ridge.
TABLE OF CONTENTS

SESSION 1: GENERAL PRESENTATIONS:
NJOY-91, THEMIS AND CAENDE

Chair: John Rowlands

How to NJOY ENDF-6.
(R.E. MacFarlane) .................................................. 9

Verification of Group Constants Generated by
NJOY and CAENDE for use in ECCO.
(C.J. Dean and C.R. Eaton) ...................................... 31

SESSION 2: SPECIFIC PRESENTATIONS: ADDITIONAL
MODULES, ASPECTS OF PROCESSING
REQUIRING FURTHER ATTENTION

Chair: Cheikh Diop

Interpolation in the Unresolved Resonance Region.
(J.L. Rowlands) .................................................... 57

Approximations in the Treatment of Doppler Broadening:
Secondary Energy Distributions and Solid State Effects.
(J.L. Rowlands) .................................................... 61

Chair: Christopher Dean

TRANSX Today and Tomorrow.
(R.E. MacFarlane) ................................................ 69

An Iterative Method to Solve the Slowing
Down Equation in Homogeneous Media.
(A. Jehouani) ....................................................... 91
Chair: Caroline Raepsaet

The Monte Carlo Neutron Transport Calculation Using the Probability Table Method for Cross-sections.  
(S.H. Zheng, P. Ribon, C.M. Diop, and J.C. Nimal) ................................................. 95

Development of DRAGR for the Formatting of DRAGON Cross-section Libraries.  
(A. Hébert and H. Saygin) ......................................................................................... 103

NSLINK: A Code System to Link NJOY to SCALE.  
(P.F.A. de Leege) ........................................................................................................ 115

DRAWBS- A Graphics Output Module Basing on GKS.  
(S. Lehmann, M. Löhnte, and J.K. Axmann) ............................................................... 123

Session 3: GROUP CROSS-SECTION LIBRARIES, BENCHMARKING-APPLICATIONS

Chair: Giancarlo Panini

New Data Libraries for Fast Breeder Calculations.  
(S. Pelloni) .................................................................................................................. 135

IAEA Activities in Nuclear Data Processing for Thermal, Fast and Fusion Reactor Applications Using the NJOY System.  
(S. Ganesan and D.W. Muir) ...................................................................................... 145

Chair: Margarete Mattes

NJOY-91 and Thermal Reactor Applications.  
(A. Trkov and M. Ravnik) ......................................................................................... 171

Processing EFF-2.2 with ACER of NJOY 91.13 to Produce an MCNP Library.  
(L. Petrizzi) ................................................................................................................ 183
Session 4: USER EXPERIENCE AND PROGRAM MAINTENANCE

Chair: Doug Muir

Analysis of Neutron Deep Penetration Experiment by Tripoli Code.
(S.H. Zheng) ................................................................. 189

Heavy Nucleus Resonance Absorption in an Heterogeneous Lattice.
(M. Coste, H. Tellier, C. Raepsaet, and C. Van Der Gucht) ............ 195

Use of NJOY/THEMIS System in the Scope of the Sensitivity, Uncertainty and Data Adjustment Analysis.
(E. Kodeli) ................................................................. 199

Processing of EFF-1 Library for Tripoli Monte Carlo Code with NJOY/THEMIS System and GROUPXS Module.
(C.M. Diop, L. Giancarli, C. Raepsaet, and A. Monnier) .................. 203

NJOY to Detect Improperly Defined Data.
(D.E. Cullen and G.C. Panini) .............................................. 209

LIST OF PARTICIPANTS .................................................... 217
Session 1:

GENERAL PRESENTATIONS
NJOY, THEMIS, AND CALENDY

Chair:
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HOW TO NJOY ENDF-6*

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ABSTRACT

The new ENDF-6 format for evaluated nuclear data is being used for ENDF/B-VI in the US and for JEF-2 in Europe. The new features of the format have created opportunities to improve evaluations and to incorporate new kinds of data, but they have also created headaches for those who have to process the new libraries and use them for actual calculations. The NJOY nuclear data processing system is now able to handle most of the features used in ENDF/B-VI, and our experiences in processing this library are reported. The current status of NJOY owes much to international cooperation, and recent contributions from users around the world are reviewed. Known problems are also listed, and some new features that are needed or under development are discussed.

I. INTRODUCTION

The Evaluated Nuclear Data Files (ENDF) system has been very successful in providing high quality nuclear data to many users over the last 25 years. Each new version has introduced improvements and extensions to the formats as well as new nuclear data evaluations. The sixth and latest version contains especially ambitious changes in the formats. These changes have created opportunities to improve evaluations significantly. They also allow many new types of nuclear data to be incorporated into ENDF-format libraries. Examples of the new features include

- a reorganization into sublibraries to provide cleaner distinctions between data for different incident particles (neutrons, protons, etc.) or data of different types (decay data, fission-product yield data, thermal data);

- a restructuring of reaction naming conventions to allow for charged-particle induced reactions;

• the introduction of new resonance-region formats such as Reich-Moore, Hybrid R-Function, and R-Matrix to take advantage of modern high-resolution data, sophisticated fitting codes, and improved nuclear model codes;

• a new system for representing production yields and energy-angle distributions for all products of a nuclear reaction, general enough to take advantage of modern nuclear model code results;

• special formats for charged-particle elastic scattering that allow full treatment of nuclear scattering, Coulomb scattering, and the interference between them;

• new formats for representing the uncertainties in the cross sections and distributions included in an evaluation.

However, the introduction of new evaluations that take advantage of these features has been a problem for many users because existing applications and processing codes have to be upgraded to take full advantage of the new features. One such code is the NJOY nuclear data processing system. At its current version level of 91.34, NJOY has been able to process most of the ENDF/B-VI evaluations into pointwise and multigroup forms. Our experiences in doing this processing will be described in the following sections.

The current status of NJOY owes much to international cooperation. Users around the world have been very helpful in finding problems and suggesting solutions. Many of these contributions will be noted in the following sections. With so many NJOY installations doing active work, the procedures used for revision control and quality assurance (QA) become very important. These procedures are still under development, and their current status will be described in one of the following sections.

Finally, a code system like NJOY never seems to be finished. A number of shortcomings have shown up in the processing of ENDF/B-VI and JEF-2. In addition, there are a number of improvements that should be made to the methods used in NJOY. Some of these problems will be described in the following sections.

II. ENDF/B-VI

The ENDF/B-VI library and the first modification set to it (VI.1) have both been released and are freely available. (Please note the convention that ENDF/B-VI refers to the US library and ENDF-6 refers to the format, which is also used by other libraries such as JEF-2.) Many of the materials in the library have been
converted from earlier ENDF/B-V evaluations, and some of the new evaluations use formats that are basically the same as the ENDF/B-V format. There are no new problems associated with processing these materials.

The new materials in ENDF/B-VI that use the new capabilities of the ENDF-6 format fall into a few classes depending on where the evaluation was performed and what special features of the format were used. Especially significant are the evaluations from the Oak Ridge National Laboratory (ORNL), the Lawrence Livermore National Laboratory (LLNL), and the Los Alamos National Laboratory (LANL).

Class 1 The ORNL evaluations for $^{50-54}$Cr, $^{55}$Mn, $^{54-58}$Fe, $^{58-64}$Ni, $^{63,65}$Cu, and $^{206-208}$Pb, which use a Reich-Moore resonance representation and a lab Legendre representation for File 6 energy-angle distributions.

Class 2 The ORNL evaluation for $^{19}$F, which is similar to the class above except that it uses a special representation for the (n,2n) reaction in File 6.

Class 3 The LLNL evaluation for $^9$Be, which uses the angle-energy ordering option to describe the (n,2n)$\alpha$ neutrons and $\alpha$ particles in File 6.

Class 4 The LANL evaluation for $^{2}$H, which uses a phase-space distribution for the (n,2n) reaction in File 6.

Class 5 The LANL evaluation for $^{11}$B, which gives the distributions of secondary neutrons in File 6, but which does not have charged-particle distributions.

Class 6 The fissionable materials that use new resonance representations and/or File 6. These include $^{237}$Np, $^{235}$U, $^{238}$U, and $^{239}$Pu, with contributions from LANL, ORNL, and Harwell.

Class 7 The LANL translations of the old ENDF/B-III thermal moderator evaluations into ENDF-6 format.

III. POINTWISE PROCESSING

The normal procedure used for ENDF/B-VI processing at Los Alamos starts by breaking up the ENDF "tapes" received from the National Nuclear Data Center at the Brookhaven National Laboratory into separate materials and storing them in a hierarchical storage system with paths like "/endf/6/neutron/u/235" or "/endf/6/thermal/h2o." Clearly, the third field is the ENDF-6 sublibrary name, the fourth is the chemical name, and the last is the isotope name (or "nat"). Each of these material files is then sent through the sequence of NJOY modules RECONR, BROADR, UNRESR, HEATR, and THERMR to generate a pointwise version of the material. These so called "PENDF" files are stored in the
file system using paths like "/pendf/6/u/235." Problems introduced by ENDF-6 occur mostly in resonance reconstruction, heating and damage calculations, and thermal-scattering calculations.

A. Resonance Reconstruction

Processing logic for the Reich-Moore resonance representation was included in NJOY 89, and it was checked against the SAMMY code\textsuperscript{6} used to prepare Reich-Moore resonance tabulations at Oak Ridge and against other codes during the code comparisons exercises initiated by D. E. "Red" Cullen when he was at the IAEA. These exercises are now being continued by Srinivasan Ganesan during his tenure at the IAEA Nuclear Data Section. Careful studies of the results of resonance reconstruction using RECONR by Ganesan hinted at some problems. Further studies by Cullen and by Eaton, Dean, and Rowland at Winfrith revealed two errors:

- Duplicate J values were being treated incorrectly in the Reich-Moore section. This resulted in incorrect values of the potential scattering cross section. It was fixed in version 91.2 using a patch supplied by Charles Dunford of the National Nuclear Data Center.

- An incorrect channel radius was being used in connection with the NAPS=1 option for Reich-Moore parameters. This resulted in incorrect peak cross sections for resonances in material like $^{56}$Fe. It was fixed in version 91.15 using code contributed by Winfrith.

Several other small changes were made in RECONR, including patches submitted by Margarete Mattes of U. Stuttgart, Caroline Raepsaet of CEA, and Gian Carlo Panini of ENEA Bologna.

The current version of the RECONR module (91.28) has been used to process all of the materials in ENDF/B-VI successfully. However, there are still several improvements that need to be made:

- Improve accuracy on short-word machines. Current methods allow 7 digits of accuracy on Sun or VAX, but only six on IBM machines. There are energy regions where as many as 8 significant digits might be necessary.

- Repair the Hybrid R Function representation. Problems have been reported by Harold Knox of Westinghouse when processing the new ORNL evaluation for Si-28.

- Add coding to handle the Generalized R-Matrix formalism. This may be needed for high-quality light-isotope evaluations in the future.
• Process resonance parameters to produce detailed angular distributions in
the resonance range. This step is possible using the new evaluations from
ORNL, and improved angular distributions might be important for deep-
transport problems.

B. Heating and Damage

A number of the new features of the ENDF-6 File 6 were chosen to improve
the calculation of nuclear heating (KERMA) and radiation damage (or DPA),
which was very difficult with earlier versions of the ENDF libraries because of
energy-balance problems.\textsuperscript{7,8} These earlier versions of ENDF did not have the
explicit distributions for the emitted charged particles, including the recoil nu-
cleus, that are allowed in ENDF-6. Thus, it was necessary to compute the energy
deposited in charged products by subtracting the neutron and photon energies
from the energy available. This procedure requires extraordinary accuracy in
maintaining energy conservation for all parts of the evaluation because these
differences are often relatively small. Modest problems with interpolation and
problems determining the effective available energy for elements would often be
magnified into negative or absurdly large heating values.

However, the charged particles can be represented explicitly in an evaluation
using ENDF-6. It is then straightforward to obtain the heating by summing up
the contributions from all the particles for each reaction. These distributions are
normally calculated using nuclear model codes, and an example of the kind of
improvement obtained for the ORNL evaluation of copper is shown in Figure 1.
(The elemental heating value from the isotopic values for \textsuperscript{63,65}Cu with the new
MIXR module available in NJOY 91.)

The HEATR runs went well for the materials in Class 1 and 2, which have very
complete File 6 data that were explicitly adjusted to conserve energy for every
reaction. The dramatic improvements in the heating cross sections provided by
these ORNL evaluations for the important materials of iron, nickel, chromium,
copper, and lead is one of the major advantages that ENDF/B-VI has over its
predecessor. The HEATR runs also went well for \textsuperscript{9}Be because HEATR is able
to process the secondary distributions for the \textalpha particles given in the "Law 7"
ordering \( E, \mu, E' \). Similarly, \textsuperscript{4}He in Class 4 was easy to process because the energy
of the secondary proton from the \((n,2n)\) reactions is determined by the phase-
space law used in File 6.
Figure 1: KERMA comparison for elemental copper in ENDF/B-VI (solid) and ENDF/B-V (dashed). The improvement was made possible by using a nuclear model code to do careful evaluations for the individual isotopes and by using File 6 to give the distributions for all charged reaction products.

The case of $^{11}$B from Class 5 was more difficult. This material contains a File 6 description of the emitted neutrons, but the subsections for charged particles and the recoil nucleus were not included. HEATR drops back to using an energy-balance calculation. A future revision will remove this fault.

Because the heating for the materials in Class 6 is dominated by fission, accurate treatments of recoil from other reactions is not very important. These evaluations describe only emitted neutrons in File 6, and HEATR uses energy-balance to obtain the KERMA.

The final results of running HEATR on the materials of ENDF/B-VI have been reported elsewhere. In general, the results were very good for ENDF/B-VI materials that use File 6, but many materials carried over from ENDF/B-V and some of the materials evaluated for ENDF/B-VI that don't use File 6 have significant energy-balance problems.
C. Thermal Scattering

The ENDF-6 format for thermal scattering data contains a few extensions to include subsidiary data that was missing from the original format (such as effective temperatures for the short-collision-time approximation), and a better representation for coherent elastic scattering. The old ENDF/B-III thermal evaluations were converted to ENDF-6 format at Los Alamos, but no new physics was added. It was fairly easy to process the ENDF/B-VI data using the THERMR module of NJOY 91. Some small corrections were necessary, including contributions from Mattes to fix some problems with cold moderators. Chris Dean of Winfrith, Fortunato Aguilar of ININ, and Uli Decher of Combustion Engineering submitted patches for short-word machines. The current level of THERMR is 89.22.

The only significant problem found during thermal processing is that the coherent elastic data for graphite in ENDF/B-VI is incorrect above 0.1 eV. We hope to fix this soon and to make other improvements to the ENDF/B-VI thermal evaluations.

IV. MULTIGROUP PROCESSING

Multigroup cross sections and transfer matrices for nuclear reactions are produced by running the GROUPR module of NJOY with a particular group structure, weighting function, Legendre order, temperature list, and $\sigma_0$ list. At Los Alamos, we write out the results in our file system using paths like /lib30/6/gendf/u235 and /lib30/6/output/u235. As of this date, we have been able to process most of the materials from ENDF/B-VI and VI.1. Table 1 summarizes our work. After all the materials needed for a library have been processed, they are assembled into a MATXS library using MATXSR.

The only ENDF/B-VI material that we have not been able to process is $^{19}$F, which uses an unusual representation for the ($n$,2$n$) reaction in File 6. Two subsections are given for emitted neutrons, one for the first neutron, and one for the second. NJOY cannot currently handle this option, and we have substituted the ENDF/B-V version of $^{19}$F into our libraries for the present.
Table 1: Number of ENDF/B-VI and VI.1 materials that have been processed into various libraries at Los Alamos. The notation “30×12” means 30 neutron groups and 12 photon groups.

<table>
<thead>
<tr>
<th>Library</th>
<th>Groups</th>
<th>Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>matxs10</td>
<td>30×12</td>
<td>117</td>
</tr>
<tr>
<td>matxs11</td>
<td>80×24</td>
<td>95</td>
</tr>
<tr>
<td>matxs12</td>
<td>69×24</td>
<td>140</td>
</tr>
<tr>
<td>matxs13</td>
<td>187×24</td>
<td>32</td>
</tr>
<tr>
<td>matxs14</td>
<td>175×42</td>
<td>32</td>
</tr>
</tbody>
</table>

A. Constant Spectra

The most significant change made in GROUPR recently was started in 89.63 (June 1990). For low incident neutron energies, the shape of the neutron and photon spectra from fission and the photon spectrum from radiative capture does not depend on energy. As a result, a fission matrix for a large group structure with many thermal groups (such as our 187-group structure) contains much redundant information. Large amounts of time and storage space can be saved by decomposing such matrices into the sum of a product of two vectors and a smaller matrix. GROUPR does this automatically by determining the energy range in which the spectrum shape will be constant from the ENDF file. It then computes a single spectrum, giving the fraction of neutrons or photons appearing in each energy group for reactions caused by neutrons in this energy range. GROUPR also computes a production cross section for each incident-energy group that lies in the constant range. The transfer matrix is then computed for incident-energy groups above the constant range and all secondary-energy groups. As an example, a 187×187 fission matrix might decompose into a 187-group spectrum, a 132-group production cross section, and a 53×187 matrix for a savings of 70%. The spectrum and production cross section are added to the section in the GENDF file for the matrix. The trick is to give the spectrum as a record with IG=0 and to give the production cross section as a set of records for the low-energy groups with IG2L0=0.

The problem with this improvement is that its effects propagate into all the other NJOY modules that use GENDF input; namely, MODER, DTFR, CC-CCR, MATXS, POWR, WIMSR, and PLOT. The effects were most signifi-
cant for MATXS. It was necessary to modify the MATXS format to allow all
the details of these decomposed matrices to be preserved. This, in turn, causes
problems for codes that use MATXS input like TRANSX and BBC.\textsuperscript{13}

B. MATXS Changes

The necessity to make one change to the MATXS format created the oppor-
tunity to make other changes. One of the problems with the original MATXS
format was that it was difficult to insert a new material or replace an old material
in an existing library. This was due to the organization of the library by "data
types." All the neutron scattering data for all materials was stored together,
followed by the photon production data for all materials, and so on. We decided
to change the organization so that all data types for a given material were stored
together, followed by all data types for the next material, and so on. This made
it much easier to write a version of the BBC library-maintenance code with the
following advanced capabilities.

- Insertion of one or more new materials at any point in the library.
- Deletion of materials.
- Replacement of any material with a new version.
- Extraction of a subset of the materials on a library to make a new smaller
  library.
- Listing, indexing, and conversion between binary and BCD modes.

The extraction option can be used to speed up TRANSX runs for a class of
problems by reducing the amount of data TRANSX has to read for each run.

C. Other GROUPR Changes

Other changes to GROUPR include some new group-structure and weight-
function options, several small repairs to the coding (thanks are due to Peter
Laughton of AECL Canada and to Caroline Raepsaet of CEA-DMT Saclay for
some of these), a number of improvements to the flux calculator developed at
Los Alamos or suggested by John Rowlands (Winfrith and Cadarache), and
an update to allow tabulated angular distributions in File 6 contributed by M.
Konieczny of the Culham Laboratory.
The current list of future projects for GROUPR follows.

- Fix File 6 processing to allow multiple subsections for an emitted particle. This option is found in ENDF/B-VI $^{19}$F.

- Fix File 5 processing to allow multiple tabulated emission laws for a neutron. This case is found in JEF-2. A draft update for this problem is available (Dean, Winfrith).

- Repair some problems in the treatment of charged-particle elastic scattering reported by Vontobel of the Paul Scherrer Institute.

V. MONTE CARLO PROCESSING

The capability to prepare ENDF-6 evaluations for use by the Los Alamos Monte-Carlo code MCNP$^{11}$ has been delayed significantly beyond our original targets, and neither NJOY nor MCNP are currently able to take full advantage of the new evaluation in ENDF/B-VI. Part of the problem is that the effects of ENDF-6 features propagate throughout the entire system. MCNP has to be changed to take advantage of File 6 distributions, the ACE format has to be changed to deliver the data to MCNP, and the ACER module of NJOY has to be changed to prepare the new ACE file. The following were our targets:

- MCNP should be able to sample from all the neutron energy-angle distributions available in File 6.

- MCNP should be able to sample from all the photon production data, whether given in the old File 12/13/14/15 style or given in File 6.

- MCNP should have a full probability-table treatment available for unresolved region cross sections.

- MCNP should be able to handle the extremely large tabulations of resonance cross sections found in some of the new ENDF/B-VI evaluations.

- The ACER module of NJOY, which is used for producing ACE-format libraries for MCNP, should be improved so that it could be used more easily away from Los Alamos.

We started this process with a major update to ACER in version 89.60 in May of 1990. This version was intended to attack the last target in the above list. It broke up the large subroutines into smaller ones, handled many Hollerith/character data type problems, solved many problems arising from mixed real and integer data in arrays, and provided capabilities to work with Type 1, Type 2, and Type 3 libraries. It also added a capability to produce ACE
dosimetry files, and it added the first part of a new capability to produce ACE photoatomic files.

Of course, a massive change like this is hard to do without making mistakes and omissions. We found a number of them on our own, and many others were kindly reported to us by Margarete Mattes of U. Stuttgart, Peter Vontobel of the Paul Scherrer Institute, and Max Lazo of SAIC/Albuquerque and the Sandia National Laboratory (SNL). These changes will mostly be found in version 91.25 dated 6 December 1991.

A. Using File 6 in MCNP

It still remained to attack the first three targets in the above list. ACER in NJOY 89 already had limited capabilities to work with File 6 if the Kalbach law was used to represent the energy-angle distribution for the emitted neutrons. It also had the capability to extract photon production data from the sections of File 6 and to write it into the ACE file using the existing “detailed photon production” format. The ACE format for this data was called “Law 44.” A patch existed for MCNP that allowed the code to sample from the neutron energy-angle distributions and from the detailed photon-production data. However, we were not able to work with the energy-angle-energy representation used in the LLNL evaluation of $^9$Be, with the lab Legendre representation used in the ORNL evaluations, or with the phase-space representation used for the (n,2n) reaction in $^2$H.

Some work was done on the $^9$Be case in early 1991 by Bob Seamon and Bob Little at Los Alamos. They defined a new ACE format for the data, prepared the cross sections in the new format, modified MCNP to sample from the new data, and tested the entire package. The ACER module of NJOY has not been upgraded to prepare this new format as yet. No work has been done in either MCNP or NJOY for handling the phase-space distribution used by the ENDF/B-VI evaluation for $^2$H.

A more important need is the ability to handle the ORNL evaluations for important materials like iron, the components of stainless steels, copper, and lead. These evaluations give the energy-angle distributions for secondary neutrons as laboratory Legendre expansions for each $E \rightarrow E'$ transfer. It is difficult for a Monte-Carlo code to sample from the Legendre distribution, but it is easy to sample from the Kalbach distribution. This suggests that one should convert
the Legendre data into an equivalent Kalbach function. If the Kalbach formula really provides a universal function for representing these angular distributions (as it claims), the converted distribution should be as good or better than the original one (better because truncation oscillations in the Legendre expansion would be eliminated). Methods for making this conversion have been developed by Arnie Sierk at Los Alamos and included in version 91.32.

Basically, Kalbach claims that the angular distributions in the center-of-mass for emitted particles can be represented well by the the function

$$f(\mu) = \frac{a}{2\sinh(a)} \left[ \cosh(a\mu) + r \sinh(a\mu) \right],$$

(1)

where $a$ is a simple function of mostly $E'$, and $r$ is the preequilibrium fraction. When $r=0$, evaporation dominates, and $f(\mu)$ is an even function. When $r=1$, preequilibrium processes dominate, and $f(\mu)$ shows a strongly forward-peaked behavior. Our method starts with the angular distribution from the ORNL evaluation and computes the values of the forward and backward scattering in the CM frame. The parameters $r$ and $a$ are then chosen to reproduce these two values. A typical example of the type of fit obtained is shown in Figure 2. The functions $r(E, E')$ and $a(E, E')$ that result from this process are written out on the ACE file using Law 44 just as if the original evaluation had used the Kalbach representation.

The advantage of this approach is that no additional changes have to be made to MCNP or the ACE format. The large set of new evaluations from ORNL is immediately available to the MCNP user.

B. Using Probability Tables in MCNP

The second and third targets in our original MCNP list can both be attacked by using probability tables. ENDF evaluations represent the unresolved-resonance range by giving average resonance parameters and specifying the distribution function for each of the parameters. In RECONR, these parameters are used to compute the expectation value for the total cross section as it would be observed in a thin sample or a dilute mixture. In the past, only this infinitely-dilute cross section has been made available in ACE libraries. Thus, the effects of self-shielding in the unresolved range, which are important in many applications, have been neglected by MCNP.
A number of years ago, Lee Carter of the Hanford Engineering Development Laboratory (HEDL) developed a patch to allow MCNP to use the probability table method pioneered by Levitt. 12 Jacek Arkuszewski of the Paul Scherrer Institute also worked on this patch during and after a visit to Los Alamos. The method is based on the following argument. If the width of the resonances is small with respect to the average energy loss in scattering (the NR approximation), neutrons appear in a given energy range with energies that are not correlated with the positions of resonances in that range. The probability of that neutron seeing any particular value of the cross section can then be chosen randomly from the appropriate distribution, or "probability table." We developed the PURR module of NJOY to produce the probability tables from ENDF evaluations. Bob Little of Los Alamos developed the methods to patch the results of PURR into MCNP. Unfortunately, this technology has never been developed to the point at
which it can be included as a standard part of the MCNP system. This final step needs to be made in the near future.

In preparation, we have recently made a major upgrade to PURR. The main feature of this upgrade is to treat all the temperatures at once in order to preserve the correlations in the cross sections. This means that a neutron that samples a particular cross section in a region at temperature \( T_1 \) will see a related cross section if it travels into another region where the temperature is \( T_2 \). PURR now writes all its results on the PENDF tape using a specially defined format in File 2 with MT = 153. ACER has been modified to watch for this section. Additional coding must still be added to extract the probability tables from the PENDF tape and to load them into the ACE file.

Several of the evaluations of ENDF/B-VI have dramatically improved their resonance representation by pushing the boundary between the resolved and unresolved range to higher energies. For example, the ENDF/B-V evaluation of \(^{235}\text{U}\) used a breakpoint of 82 eV, and the new ENDF/B-VI evaluation uses 2.5 keV. This means that a very large number of energy points are needed to represent the resolved-energy range on the PENDF file. These huge resonance tabulations can load down MCNP and make library transfer and storage very expensive, especially when workstations are used to run MCNP instead of large supercomputers. The obvious way to alleviate this problem is to convert the high-energy part of the resolved-range tabulation into probability tables that use the same format as the unresolved-range tables produced by PURR. These tables can then be used by the existing unresolved patch for MCNP. As long as the NR approximation conditions used to justify the probability table method remain valid, this step of converting point cross sections into probability tables should cause little degradation in the accuracy of the MCNP results.

The mechanics of converting point cross sections to probability tables have been developed for the probability-table option of TRANSX.\(^{13}\) The next step is to incorporate these methods into ACER as a thinning option, and to link the results into the ACE file as if they had come from PURR.

C. Developments Needed for Monte Carlo

The additional developments still needed for MCNP and the Monte-Carlo part of NJOY are listed below.
• Add a capability to sample from phase-space distributions to MCNP and add an appropriate format to the ACE file specifications.

• Add coding to process phase-space distributions and the type of distribution used for $^9$Be to the ACER module of NJOY.

• Add coding to copy the probability tables from MT153 on the PENDF tape into the ACE library. Also provide code to print on the output listing.

• Add an additional thinning method in ACER, which will convert high-energy resonance cross sections into probability tables, write them on the ACE file, and print them on the output listing.

• Finish the photoatomic section of ACER by providing a method of producing tables of fluorescence photons and electrons. MCNP may have to be modified to accept more detailed fluorescence data.

VI. PHOTOATOMIC DATA

New photoatomic data are included in ENDF/B-VI as supplied by LLNL. These data include subshell cross sections not previously included in ENDF photon interaction libraries. In addition, Livermore has recently released data on fluorescence yields and electron energy deposition that will allow the user to make accurate photon transport and heating calculations at low photon energies.

Photoatomic data are processed into multigroup form by the GAMINR module. We were able to generate libraries for the 12-, 24-, 42-group structures with no difficulty. These libraries include the basic photoatomic cross sections and matrices for coherent scattering, incoherent scattering, and pair production. Photoelectric absorption is treated as a photon disappearance reaction, resulting in local heating only. The new fluorescence data from LLNL should allow us to convert the photoelectric absorption reaction into a transfer matrix. The fluorescence photons produced by this matrix could then be transported to cause other reactions elsewhere in the system.

Photoatomic data are processed into Monte-Carlo form by ACER. The current version of the code can successfully process the cross sections and tables for coherent scattering, incoherent scattering, and pair production. The code currently ignores fluorescence. Therefore, the new cross sections would have to be merged with the fluorescence tables from the existing MCNP libraries to be useful at this time. The next step would be to redesign the fluorescence treatment in MCNP, the library format that supplies data for the treatment, and the coding in ACER that produces the photoatomic data in order to take advantage of the new data from LLNL.
In the existing system, MCNP handles fluorescence, but it is ignored in multigroup calculations. This sometimes leads to noticeable differences between Monte Carlo and $S_N$ results. The steps outlined above would remove this shortcoming from the multigroup libraries and improve the Monte-Carlo libraries in such a way that the two different kinds of calculations would be consistent.

VII. PLOTTING

The ability to make good, publication-quality graphs of nuclear data is very important. It can even be considered to be a part of the QA environment, because errors are often easier to find from graphs than in any other way. However, plotting is normally very machine-dependent, and it can be very expensive to install the many systems required to deal with all codes. Luckily, a default standard is beginning to appear. Almost everyone seems to have access to a PostScript\textsuperscript{15} compatible printer these days. Many workstations (and even personal computers as small as a 386 VGA notebook) are capable of displaying PostScript graphics on their screens. In addition to being the least expensive way to display graphics, PostScript is also the best way, with the richest selection of drawing operations and fonts of any system.

Therefore, we have decided to modernize and unify the graphics sections of NJOY by supplying the output in PostScript format. The main principle used to design computer codes that are easy to transport to other systems is to push the machine-dependent parts to as low a level as possible. For example, most of the machine-dependent coding is NJOY is contained in a few subroutines in the NJOY section of the system. The ultimate extension of this principle is to push the plotting work entirely out of NJOY. The system currently contains three modules that produce graphics.

**DTFR** This module draws its own axes and characters based on fairly old methods. It has had the advantage of being easy to adapt to other systems because the interface is on the vector level. The results are not publication quality.

**COVR** Fairly nice shaded contour graphs of the correlation matrix and graphs of the variances along both axes are produced using DISSPLA.

**PLOTR** This module can generate a number of two-dimensional and three-dimensional plots of ENDF, PENDF, GENDF, as well as experimental data, including overlays of different curves and flexible titles, curves tags, or legends. DISSPLA is used; the results are close to publication quality.
Although DISSPLA\textsuperscript{16} is available at a number of the larger computer centers, not everyone has it. In addition, it is very expensive to install on workstations, and it is possible to produce better quality output with the less expensive PostScript approach.

Our first step has been to convert the PLOT module of NJOY into a stand-alone code that reads a simple text input file similar to the current PLOT input for experimental data and produces the plots directly in PostScript format. These PostScript files can then be sent to a printer, or they can be viewed on a screen if you have suitable software. The next step is to modify each of the three NJOY modules listed above to write the text interface file instead of generating graphs directly.

When this process is finished, NJOY will not contain any graphics calls at all, and all the complexities associated with mounting graphics libraries will be gone. The stand-alone PLOT module can be used to produce plots in PostScript, or it could be modified to use other systems such as GKS. In fact, we have a version that has been converted to C and equipped with an OpenLook window system. This allows graphs produced by NJOY to be viewed and modified using the mouse on a Sun workstation.

VIII. REVISION CONTROL AND QA

Nuclear cross sections are needed in many programs that are forced to operate under strict Quality Assurance (QA) procedures. Although “grandfather” clauses have allowed existing code systems like NJOY to be used in QA environments, there are strong pressures to make NJOY comply with QA rules. There are a number of different formal QA documents currently available, such as the US national standards published by the American National Standards Institute and the Institute of Electrical and Electronic Engineers (ANSI/IEEE series), the DOE NQA series for nuclear activities (DOE Order 5700.6c, “Quality Assurance”), and even local versions such as the “Los Alamos National Laboratory Quality Assurance Manual.”

All of these various standards share some common principles, one being that is necessary to carefully control changes to computer codes in order that it always be possible to determine exactly what version was used for any given task. This principle has the following four components:
• A history of all the changes to the computer code that allows its state at any particular time to be reconstructed.

• Labeling of code listings and job output listings that allows the version used for any task to be determined.

• Documentation of the reasons for and results of each set of changes to the code.

• Protection of source code and change history records against loss, damage, or tampering.

The last two jobs can only be performed by the people who maintain the code, and strict administrative guidelines are often established to make sure that the jobs are performed. The first two tasks (and some aspects of the third) should be delegated to a computer code.

A number of such codes have been used in the past in the nuclear industry. The UPDATE code\textsuperscript{17} is widely available on CDC and Cray systems, and the similar HISTORIAN code\textsuperscript{18} can be purchased for a number of computer systems. The problem with these commercial systems is that no one code is available universally, and there is no uniform “update” system that all users can be expected to have. If the system is not uniform, it is difficult to send out modification sets and have a reasonable hope that they will be used correctly by everyone. For the NJOY 89 distribution, we tried to solve this problem by including an UPDATE emulator.\textsuperscript{19} Unfortunately, this code attempted to emulate so many of the features of UPDATE that it became fairly complex and hard to port to different machines. In addition, the line numbering sometimes came out differently on different machines, especially for updates made on top of previous updates.

In order to solve these problems, we have designed a new UPDATE-type code for NJOY 91 called UPD.\textsuperscript{20} By leaving out many of the features of its ancestor, we have been able to make UPD so simple that it is easy to port to any computer. UPD works directly on the code's “source” file using a file of update “idents” similar to the ones used with the UPDATE system. There is no equivalent to the binary program libraries used by UPDATE and HISTORIAN. UPD produces compiler input files (CPL) and special listing files (LST) directly.

The UPD code is used together with a detailed revision procedure to provide history information, version labeling, and limited modification comments. A typical example of an UPN file to modify NJOY 91.0 might look like this.
The first line requests that a compiler input file (CPL) be produced. The second tells UPD to activate the short-word options (SW) contained in *IF SW... constructs in the source code. The third line starts a set of code modifications. The first set of updates must be called UP1, and it advances the version number of the code from 91.0 to 91.1. The first line (or lines) in the "ident" must be a comment that gives the name of the module, the date, and a description of the change in exactly the style shown. Using this style enables one to scan for changes with a text editor. The ident called VERS must be present. It changes the version and date comment on the source listing, and it changes the VERS constant that is used to label the output listings from NJOY. Note that these procedures satisfy the "history" and "labeling" requirements discussed above as necessary for any QA environment, and the comment card satisfies at least part of the "documentation" requirement.

If you should need to change the size of the container array in BROADR again at some later date, you cannot simply go back and edit the lines in ident UP1. This would destroy the history and make it impossible to determine the exact configuration of the code that was used on any particular date. Instead, you would add a new ident, for example UP2, that refers to line numbers like UP1.4 and UP1.6 instead of BROADR.101 and BROADR.106.

Of course, users are free to use their own schemes for numbering experimental or local changes to NJOY. When an experimental update has been finalized, it can be sent to Los Alamos for incorporation into a future release. We will periodically release "minor" versions, such as 91.13, 91.34, etc., and when the update set gets too large, we will release a new "major" version, such as NJOY 93.
IX. CONCLUSIONS

The NJOY code has been used successfully to produce multigroup nuclear data and photoatomic data from ENDF/B-VI, and it is almost ready to be used to generate libraries for the MCNP Monte-Carlo code. Thanks to generous cooperation from the users of NJOY, the code is gaining reliability and new capabilities. In addition to those mentioned in the text, the following people have contributed recently: Harm Gruppelaer (ECN/Petten), Fred Mann (Westinghouse Hanford), Clas Grägg (Studsvik), Mike Milgram (Chalk River), Ian Gauld (Whaleshell), Doug Muir (IAEA), Claes Norborg (NEA-DB), and Enrico Sartori (NEA-DB). Finally and specially, Denise George of Los Alamos has made major contributions to the success of the NJOY processing system.

X. REFERENCES


18. HISTORIAN is a product of Opcode, Inc., P. O. Box 10998-537, Austin, TX 78766-1998.


Verification of Group Constants Generated by NJOY and CAENDF for Use in ECCO

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Summary

This paper briefly describes the generation of nuclear data for the European Cell Code ECCO. It shows how the codes NJOY and CAENDF are applied. As the data are taken from more than one code, it is important to check that the data are both correct and consistent. The code Merge amalgamates the output from both codes. The code CRECCO writes the group constants to the ECCO nuclear data library. Both codes perform many checks which are described. As a result of these checks improvements have been made to NJOY, CAENDF and the JEF2 evaluated nuclear data. Examples are given. We conclude that the Quality Assurance of the nuclear data in the ECCO libraries is greatly enhanced by the use of these checking tools.
1. Introduction

In the framework of the European Fast Reactor Collaboration (1) the core physics programme (AGT3) includes a project to generate a common cell code called ECCO (2). ECCO requires multi-group cross sections in fine ($\Delta_{u}=1/120$) and broad ($\Delta_{u}=1/2$) energy groups. This paper firstly describes how these data are generated. It then specifies the role of NJOY (3)/THEMIS (4) and CALEND$F$ (5) in generating the required group constants.

NJOY and THEMIS output group data on a GENDF file. CALEND$F$ has its own output structure. The MERGE code is used to add CALEND$F$ output to the GENDF to form a GENDF$^*$ file. During this operation common data generated from both codes are processed and compared.

The data on the GENDF$^*$ are added to the ECCO library by the CRECCO code. This performs several consistency checks.

The main purpose of this paper is to describe the checks performed by MERGE and CRECCO. It then demonstrates through examples, how the checking procedure has highlighted problems in NJOY, THEMIS, CALEND$F$, and in the JEF2 evaluated data. The paper shows how NJOY/THEMIS have been used to check CALEND$F$ and vice versa. It also shows how, by processing ENDF/B-6 format data with two different codes, one can help improve the evaluated data.

2. ECCO Data Generation

2.1 Quantities Required

ECCO requires neutron cross sections and scatter matrices covering the energy range 20 MeV - 1.0E-5 eV. It is intended to use ECCO for fast reactor calculations but an ability to study slowing down spectra in the resonance region to help validate thermal reactor methods has necessitated the production of low energy data. Libraries of fine group ($\Delta_{u}=1/120$) constants are generated for the more important nuclides for use in reference calculations. Broad group ($\Delta_{u}=1/2$) libraries are generated by consistently condensing the fine group data using a code called CONDEN$A$. Data for less important substances are generated and added to this library.

Primary cross sections are defined as those needed by ECCO to calculate neutron fluxes and components of neutron balance. (e.g. total, transport, $\nu$-fission and capture). Four of these lead to neutron sources. Scattering matrices (up to P5 for reactor shielding purposes) are needed for elastic (fast and thermal), inelastic (high energy), and $n$,Mn (the summation of all multi-neutron production except fission). Fission spectra are required for each fissionable nuclide and can, if desired, be specified at particular incident neutron energies. Response functions include the potential for such items as KERMA, displacement cross sections, and isotope activation. In addition gamma source data for capture, fission and inelastic are desired.

Resonance self shielding in ECCO uses sub-group probabilities and cross sections because they can be used explicitly in calculations for complex geometries whereas “Bondarenko” shielding factors require equivalence relationships to be formulated.

2.2 JEF2 Library Generation

The writing and testing of ECCO has made use of the FGL5 (6) library which was generated from the United Kingdom Nuclear Data Library - UKNDL (7). Meanwhile methods for generating new libraries based on JEF2 (8) have been developed. These were described at the last NJOY seminar (9) and at PHYSOR (10). Figure 1 shows the overall generation route. We are generating data in 1968 energy groups so all generation must be automated and checked. The function of each module in the generation route will be explained in the sections below. It can be seen however that the cross sections and scatter matrices generated by NJOY/THEMIS are joined to the resonance shielding sub-group data from CALEND$F$ by the MERGE code. The infinite dilution cross sections are produced by both codes and can be compared with a tolerance. The sub-group data can be reformatted into
Bondarenko shielding data at fixed backgrounds and similarly compared. The joined and adjusted data must be inverted in energy before being added to the direct access ECCO library.

The numbers following module and data names indicate the current versions. In the case of NJOY89.62 the extra "w" indicates the presence of local enhancements. These have all been made available to R.McFarlane for inclusion in NJOY91 and to THEMIS programmers (11).

Within the unresolved resonance region the data from NJOY cannot be compared directly with that from CALENDF. The UNRESR module of NJOY generates shielded cross sections using an analytic method. The CALENDF code generates sub-region ladders. Group data at the 1/120 lethargy level will not compare. However at the 1/2 lethargy level the random structure from the ladders should "average out" to the accuracy required. Therefore the generation route is extended as in Figure 2. The UNRESR module outputs a PENDF file containing the shielded cross sections at energy points. In Figure 1 these were averaged into 1/120 lethargy width cross sections. A second GROUPR run can thus be appended to produce 1/2 lethargy data using the same weighting function. The CALENDF code has generated sub-group resonance shielding data in the 1/120 lethargy structure. These are used to form moments of the total cross sections which are condensed in the COLLAPSE code. COLLAPSE refits sub-group parameters to these moments. A second MERGE run can then be made but this time only the checks are of interest (The joined file is not kept).

At Winfrith JEF2, and all other ENDF/B format libraries, are split into "tapes" each containing the evaluation for a single nuclide. The files are maintained as compressed 80 byte records. This allows the UNIX "uncompress" command to be used to create files for either scanning or processing without significant delay. The generation route in Figure 1 (and Figure 2, if unresolved data are present) is applied to each nuclide.

3. Role of the Processing Codes

3.1 NJOY/THEMIS

NJOY is used to generate components of infinite dilute primary cross sections, scatter matrices and response functions. Bondarenko shielded cross sections are only generated for checking purposes and are not used on ECCO libraries. No use is made of NJOY's output modules (except MODER). The CRECCO code is used to form all quantities on the ECCO library from the components. NJOY does not generate sub-group resonance self shielding factors.

The NJOY modules used are:-

- MODER - to transform the mode of ENDF, PENDF files between formatted and unformatted as needed.
- RECONR - to process resonance parameters to form 0K files on a unified energy grid.
- BROADR - to Doppler broaden the files to temperatures between 293.16 and 5700K.
- THERMR - to generate free gas thermal scattering data.
- HEATR - to generating components of heating and damage for use in response functions (not used in the current libraries).
- UNRESR - to form shielded point data in the unresolved resonance region.
- GROUPR - to form group cross sections and scattering matrices.

Thermal scattering data for bound isotopes (so far H in H₂O) are generated by inputting PENDF files, processed by M Mattes at IKE Stuttgart, into the GROUPR module. These files are being released as part of JEF2.2.
NJOY89.62 has been installed using double precision on SUN4 workstations at Winfrith (12). We make use of the -r8 option of the SUN FORTRAN 77 compilers to allow double precision INTEGERS and REALS. Initial studies (13) made use of TOOLTIP facilities (14) to automate double precisioning of the source code. The double precisioning took about one week for MODER, RECONR, BROADR, UNRESR, THERMR and GROUPR. The resultant coding was very different from the initial international source. We thus rejected the TOOLTIP method because we could not install or send out internationally compatible UPDATE changes. However TOOLTIP or similar automated tools would be valuable to the NJOY authors if revised modern source coding is to be generated and released.

We needed to use double precision in order to generate point cross sections to 0.1% (ERR=0.001) with 9 significant figures. These tolerances are needed to represent the higher energy resolved resonances in many of the JEF2 files (particularly U238). The results of our precision studies and all other changes have been made available to co-workers at Saclay. Therefore the ECCO libraries generated at Cadarache using THEMIS should be consistent with those generated using NJOY at Winfrith.

3.2 CALENDIF

CALENDIF is used to generate infinite dilute primary cross sections and sub-group resonance self shielding factors. Reactions processed are: TOTAL, ELASTIC, TOTAL INELASTIC, (n,Mn), FISSION and PARASITIC ABSORPTION. In later sections these are referred to as the “CALENDIF reactions”. As the code mainly considers resonance region nuclear data, processing of many different sub-components of these reactions is not performed, e.g. (n,2n), second chance fission, inelastic levels, (n,p) and (n,oo). However all reactions on ENDF/B-6 files are included within one of the six reactions processed. Also the TOTAL cross section is the sum of all partials. Scatter matrices, fission spectra, the mean number of emitted neutrons/fission and response functions are not generated by CALENDIF.

CALENDIF is able to process JEF2 files containing resonance parameters and PENDF files from NJOY. It has its own resonance reconstruction procedures in the resolved resonance region and sub-range ladder generation in the unresolved region. Doppler broadening to one temperature is also considered. Therefore to generate ECCO data six runs have to be made. Each operates on the ENDF/B resonance parameters.

A noticeable difference in principle between NJOY and CALENDIF is applied during the processing. CALENDIF users specify a single accuracy to which they require their sub-group constants. A linked accuracy for resonance reconstruction and Doppler broadening is formed. Resonances are reconstructed using “the best” formalism determined by the resonance spacing (usually Reich-Moore) rather than the formalism specified by the evaluator. Related accuracy is applied to reconstruction of different categories (f states) of resonances. Cubic interpolation is assumed to apply between points.

NJOY users can specify an accuracy for each processing stage. Resonances are reconstructed using the formalism specified by the LRF trigger set by the evaluator. This assumes the evaluator has fully considered all approximations involved in using the representation, e.g. multilevel Breit-Wigner. Cross sections are reconstructed using the evaluators' interpolation scheme. This excludes cubic interpolation. The final energy grid for point data is unified between reactions and fine enough to allow trapezoidal integration on a linear scale to form group constants.

In generating ECCO libraries the JEF? resonance parameters have been fed into CALENDIF and NJOY/THEMIS. Therefore all differences in processing apply to any common constants generated. By comparing output from NJOY and CALENDIF we should highlight problems in either code and in the evaluated nuclear data file.

3.3 MERGE (15),(16)

At the early meetings to discuss the production of nuclear data for ECCO, we were faced with two main problems. We could generate all the nuclear data required using NJOY and CALENDIF. We had defined a structure for the final library and tested it using FGL5 in ECCO. How did we write the ECCO library and how did we make sure that the data were correct?
We decided to split the problem into two parts. Firstly we would join NJOY and CAENDF output and make sure the data for each reaction were consistent. Secondly we would invert the data in energy and add it to the ECCO library. At the same time we would make sure that there was consistency between the data for different reactions. The first part was fulfilled when G.Panini and P.Peerani at ENEA Bologna wrote MERGE; the second when C.Eaton wrote CRECCO at Winfrith. Both codes were used at Winfrith and Cadarache to generate libraries.

We had to transfer data between MERGE and CRECCO. As the project was international, we also had to transfer data between establishments. The structure of the GENDF from NJOY was clearly defined and understood. It does not however include a specification for storage of sub-group data. We therefore consulted R.McFarlane and agreed to extend the GENDF in the manner shown in Figure 3 to give a GENDF* file. The structure for storing the sub-group resonance shielding data (MF=50) is based on that for storing cross sections (MF=3). On the first heading record, we set the number of Legendre moments (NLTP) to unity and replace the term defining the number of background cross sections by MAXNOR - the maximum number of sub-groups in any incident group. On the second, group dependent, heading record we set the number of secondary positions (NG2) to 2 to indicate the presence of a sub-group probability and a cross section. We replace the index to the next non-zero group (IG2LO) by the number of sub-groups needed in this incident group (NOR). On the record containing the sub-group data, the sub-group probability (PROB(IG)) replaces the flux and the sub-group cross section (SIGMA(IG)) replaces the background dependent cross section. We hope this format is suitable for the storage of all sub-group data generated in any future NJOY modules.

Consideration was next given as to how to make sure data are correct.

Firstly the ZA, MAT, temperatures and group boundaries from the NJOY GENDF and CAENDF's TP output files are confirmed to be equal, i.e. the user is giving MERGE the correct input data sets.

Secondly infinite dilute cross sections are formed from the sub-group parameters on the TP file thus:

\[ \sigma_R^{G}(\infty) = \sum_{g \in G} p_{g}^{G} \sigma_R^{G} \]

Where

- R indicate reactions
- G incident groups
- g sub-groups
- σ cross-section
- P sub-group probability (weight)

Similar infinite dilute cross sections for the same reactions are formed by summing appropriate data from the GENDF input file. Infinite dilute cross sections are then compared. Relative fractional group and reaction dependent ratios are stored.

Thirdly similar shielding data are formed from the sub-group parameters on the TP file thus:

\[ \sigma_R^{G}(\sigma_0) = \sum_{g \in G} \frac{p_{g}^{G} \sigma_R^{G}}{(\sigma_T^{G} + \sigma_0)} \]

\[ \sum_{g \in G} \frac{p_{g}^{G}}{(\sigma_T^{G} + \sigma_0)} \]

35
Where terms defined above apply and:

\[ \sigma_0 \] is the background cross section per atom defined in the input to NJOY

\[ T \] indicates the Total reaction

These are compared with values read from the GENDF. This time however there is no need to store the ratios.

Printed output tables are produced for groups where the relative differences are greater than a user tolerance. A summary line indicates the number of groups with differences. Only the summary line is produced for shielded cross sections. Figure 4 contains a sample output and Table 1 shows the formation of the “CALENDARF reactions” from the components on the GENDF.

The results in Figure 4 show significant differences in the UNRESOLVED resonance region. These are caused by the structure from the ladder generation in CALENDARF which is not present in UNRESR. The user is expected to ignore these differences and to check the data in this region using the method shown in Figure 2 above. If significant differences are present outside of this region they must be justified if the GENDF is to be used.

There will be small differences between the cross sections generated by NJOY and CALENDARF. MERGE has an input option to allow the user to define which data are “correct” in any energy range. Once this decision has been made all data on the GENDF must be corrected.

Corrections are formed for each of the “CALENDARF reactions”. (When NJOY is “correct” these are unity.) Relative fractional group and reaction dependent ratios are then applied sequentially to all reactions. Table 2 shows the remedial action taken when CALENDARF is deemed to be “correct”. The reaction dependent scaling is also applied to the appropriate scatter matrices. Here it is assumed that the reaction cross section is changed rather than the emergent energy distribution.

Certain improvements are needed to the actions in Table 2. For some minor reactions the production matrix is not scaled and should be. The \((n,3n+f)\) cross section and matrix should be scaled. \((n,\text{absorption})\) (MT=27) and total capture (MT=101) are rarely found on evaluations but when present they should be scaled.

Resonance self shielding is not normally applied when thermal scattering is present in ECCO libraries (below 4eV). However, if it is present, MERGE applies a correction formed using the ratio of the static nucleus elastic cross sections from NJOY and CALENDARF. This is probably suitable when the free gas model applies. For bound nuclei (e.g. C in Graphite) it assumes that the static nucleus “correction” can be linearly applied to the bound cross section and matrix. In it’s attempt to scale all thermal scattering data from both ENDF/B-IV (MT=201-230) and ENDF/B-V (MT=221-236) it ends up wrongly scaling ENDF/B-VI particle production data (MT=201-207). This should be corrected.

When NJOY is “correct” sub-group cross sections are changed to preserve the infinite dilute cross section (i.e. the change is assumed to apply to the overall cross section in the group rather than to the shape in any part of the group).

One further data manipulation can be made in a MERGE run. If the NJOY calculation requested high order \(P_n\) scatter matrices, some or all of these can be dropped for any combination of reactions. This allows data intended for reactor shielding calculations to be applied to core physics studies.

Any extra data found on the GENDF file is transferred, without change, to the GENDF. Therefore gamma source data are assumed to be correctly generated by NJOY. These are yet to be processed for ECCO libraries and MERGE will require improvement to correct these to account for changes in included neutron cross sections.

3.4 CRECO (17),(18),(19)

Having generated a GENDF file containing all the best reaction data that NJOY and CALENDARF can produce, we must add these to a new or existing ECCO direct access library. The CRECO code
performs this function by processing each reaction as it is read from the GENDF* (or GENDF). The function can, however, be divided into the following sections. Firstly make sure there is consistency between reactions at all energies. Secondly invert the data so that group 1 corresponds to high energy. Thirdly form all primary cross sections, scatter matrices, and response functions from components inverted from the GENDF*. Finally write these to the ECCO library (altering the self defining library contents at the same time).

ECCO requires Primary cross sections including sub-group resonance shielding data, scatter matrices for elastic, inelastic and (n,Mn), and various response functions. At present response functions are all individual reactions excluding total, elastic, inelastic, total fission, inelastic levels and parasitic absorption. Heating, gamma source and special response functions like total Helium production may be added later. Primary cross sections are defined thus:-

<table>
<thead>
<tr>
<th>Primary Reactions</th>
<th>Reactions Summed from GENDF* (MT's)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL</td>
<td>Sum of Primaries listed below (Inc. MThERM)</td>
</tr>
<tr>
<td>ELASTIC</td>
<td>2 or MThERM</td>
</tr>
<tr>
<td>INELASTIC</td>
<td>22, 23, 28, 29, 32-36, 51-91</td>
</tr>
<tr>
<td>n,Mn</td>
<td>16, 17, 24, 25, 30, 37, 41, 42</td>
</tr>
<tr>
<td>FISSION</td>
<td>18 (if present) or 19, 20, 21, 38</td>
</tr>
<tr>
<td>CAPTURE</td>
<td>102-109, 111-116</td>
</tr>
</tbody>
</table>

Transport and v*fission primary cross sections are also formed.

Matrices are defined thus:-

<table>
<thead>
<tr>
<th>Matrices</th>
<th>Reactions Summed from the GENDF* (MT's)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ELASTIC</td>
<td>2 or MThERM</td>
</tr>
<tr>
<td>INELASTIC</td>
<td>22, 23, 28, 29, 32-36, 51-91</td>
</tr>
<tr>
<td>n,Mn</td>
<td>16, 17, 24, 25, 30, 37, 41, 42</td>
</tr>
</tbody>
</table>

Consistency must be preserved between these types of data. The checks performed can be divided into four categories and are defined in Figure 5. It should be noted that our main function is to create a consistent ECCO library and not to fully check the contents of the GENDF*.

CRECCO has three levels of tolerance on its checks. If differences are above 1% it should stop (switched off at present) with an error message. If differences are above 0.01% a message is printed. Standard corrective action is applied to certain cross sections so that the library data are consistent.

4. Problems Encountered

The previous sections describe how ECCO libraries are produced and the verification checks used. The checks have highlighted various types of problem.

CRECCO's checks verify adjustment made by MERGE noting that both NJOY and CALENDF should preserve consistency between component and total reactions. It also checks NJOY's consistency in forming scatter matrix terms. In this latter respect we are investigating the processing of U238 inelastic continuum from the ENDF/B-VI evaluation.
At various times, the checks in MERGE have shown problems in the JEF2 evaluated data, the THEMIS installation, the physics in NJOY and in the physics in CAENDF. Most of these have now been solved but we give an example of each in order to demonstrate that the consistency checks can promote improvement in all aspects of the work.

4.1 JEF2 Evaluated Data.
The JEF2.1 file for Ni58 was based on the EFF file. Resolved resonances were represented by multilevel Breit-Wigner (MLBW) parameters. The file was processed at Cadarache using CAENDF and NJOY. MERGE results showed significant discrepancies. CAENDF had assumed Reich-Moore(RM) formalism. P.Ribon presented graphs showing the significant differences in his processing with both RM and MLBW representations. As a result M.Sowerby (20) replaced the MLBW formalism by RM for all Cr and Ni isotopes. Ironically the ENDF/B-VI evaluation for Ni58 is now included in JEF2.2 and RM parameters are present.

4.2 THEMIS Installation
After differences between CAENDF and THEMIS results had shown large differences at the boundary of resolved and unresolved resonances in U235, repeat runs with NJOY failed to show an effect.

The energy grid from the BROADR module of NJOY is recreated to a maximum of 7 significant figures by virtue of the subroutine DIGITS (11). As requests for 8 figure accuracy had been made double energy points could be seen in the file. Improvements to the THEMIS installation removed the problem.

4.3 Physics of NJOY
A large difference was seen between NJOY and CAENDF results for Fe56 capture in the 1.1497 KeV P wave resonance. The ENDF/B-VI Fe56 file was being used to compare data with JEF2.1. There had been no problem with JEF2.1 files and the CAENDF results for ENDF/B-VI were similar to those for JEF2.1. Thus NJOY's processing was suspect.

The resonance parameters in both evaluations were compared. Both files contained energy independent scattering radii (NRO=0 -see page 2.6 of reference 21) but the ENDF/B-VI file contained a trigger NAPS set to unity instead of 0. By setting NAPS to 0 the JEF2.1 file defined the channel radius “a” used in penetrabilities and shift factors by \( a = 0.123A^{\frac{3}{2}} + 0.8 \), instead of using the scattering radius. Both files contained RM parameters with different scattering radii for S and P wave resonances. The combination of NAPS=1 and “a” dependent scattering radii gave incorrect results from NJOY. Rowlands and Eaton made improvements to RECONR which were later published in reference 11.

The need to set NAPS to 1 is now in question. Tests at Winfrith indicate trivial effects on the results. Ironically the JEF2.2 Fe56 file now contains NAPS=1 as does ENDF/B-VI revision 1. NJOY, with Rowland's improvements, should give similar results for both files. These results should be similar to those obtained with NAPS=0!

4.4 Physics of CAENDF
Recent MERGE results from a JEF2 U238 calculation had shown NJOY/CAENDF differences around 10eV. These were traced to CAENDF's use of an accuracy dependent algorithm to define the energy grid. Narrow weak P wave resonances were described by fewer points than strong broad S wave resonances. Although there was some debate as to the need to represent the particular resonance by more points, study of the energy representation promoted improvements to CAENDF.

5. Conclusions
The paper shows how the NJOY and CAENDF codes have been applied for the generation of ECCO libraries. It shows how the MERGE code joins NJOY and CAENDF output. The structure of the joined
GENDF* file is described. We recommend this structure is used and enhanced for any future NJOY development with sub-group resonance self shielding data. The writing of ECCO libraries with the CRECCO code is described. Consistency checks in MERGE and CRECCO are shown to improve the evaluated nuclear data, the processing codes CALENDF, NJOY and THEMIS, and the resultant ECCO libraries.

References

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3. R.E.McFarlane
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4. C.M.Diop, C.Brienne
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   Statistical Probability Tables - CALENDF Program.
   Page 220 of the Proceedings of the Seminar on NJOY and THEMIS. Saclay, 20-21 June 1989. Published by OECD/NEA Data Bank

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11 C R Eaton, R J Perry, C J Dean
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 Installation of NJOY89.62 in Double Precision on SUN4 Workstations.

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 Progress with Processing the JEF2 Library using NJOY-89
 LWPC/P(90)5 - Internal paper

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 Numerical Algorithms Group, Oxford, United Kingdom.

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 Production of an ECCO library: the MERGE module.
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 Modifications to MERGE (Version 3)
 CFSM/P(90)115 - Internal paper

17 C.R. Eaton
 CRECCO - Code to Generate an ECCO Library from JEF Data
 CFSM/P(89)88 - Internal paper

18 C R Eaton, C J Dean
 Improvements to the CRECCO code
 CFSM/P(90)107 - Internal paper

19 C.J. Dean, C.R. Eaton, M.J. Grimstone, B. Thom
 Production of an ECCO Library from JEF-1 data
 CFSM/P(88)65 - Internal paper

20 J.B. Brisland, M.C. Moxon and M.G. Sowerby
 Resonance Region Data for Structural Materials and Sodium
 JEF/DOC - 341

21 P.F. Rose and C.L. Dunford (editors)
 ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6
Figure 1  Production of ECCO Fine Group Library from JEF2

Point Data

Cross sections
and Scattering Data

JEF2

Cross sections
and Resonance Shielding (Sub-Groups)

NJOY89-62w/
THEMIS

CALENDIF

GENDF
\[ \sigma^G_{r \sigma^G r} \]

TP File
\[ \rho^G_{\sigma^G r} \]

MERGE3.3

GENDF*

\[ \sigma^G_{r \sigma^G r} \rho^G_{\sigma^G r} \]

CRECCO

ECCO Library

Group Data
Figure 2  Extended Generation Route in the Unresolved Resonance Region

NJOY UNRESR output PENDF

NJOY GROUPR:

∞ dilute + shielded cross sections
\[ \Delta_u = 1/2 \]

CAENDF TP
file containing sub group
resonance shielding data
\[ \Delta_u = 1/120 \]

COLLAPSE code

Shielding Data
\[ \Delta_u = 1/2 \]

MERGE 3.3

Checks
### Figure 3  Structure of the GENDF

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group Bounds</td>
<td>MF = 1, MT = 451</td>
</tr>
<tr>
<td>Reaction Cross Sections</td>
<td>MF = 3, MT = 1, 2, \ldots \ldots etc.</td>
</tr>
<tr>
<td>Scatter Matrices</td>
<td>MF = 6, MT = 2, 16, 17, 51, \ldots \ldots etc.</td>
</tr>
<tr>
<td>Response Functions etc.</td>
<td>MF = 16, MT = 4, 102, \ldots \ldots etc.</td>
</tr>
<tr>
<td>e.g. gamma source</td>
<td></td>
</tr>
<tr>
<td>Sub-Group Data</td>
<td>MF = 50, MT = 1, 2, 4, 15*, 18, 101</td>
</tr>
<tr>
<td></td>
<td>Total, Elastic, Inelastic, (n,Mn), Fission, Absorption</td>
</tr>
</tbody>
</table>

* No sub-group data are kept for (n,Mn) at present.

#### Sub-Group Data Structure

The file 50 structure is very similar to that of the cross-section file (file 3). Each section starts with a "CONT" record giving:

- **ZA**: Standard Material Identifier
- **AWR**: Atomic Weight Ratio
- **NLTP**: Number of Legendre Components in Probability Tables (always 1)
- **MAXNOR**: Maximum order of Probability Tables
- **LRFLAG**: Break-up Identifier
- **NGN**: Number of Groups

This is followed by a series of "LIST" records, one for each group with available sub-group data:

- **TEMP**: Material Temperature
- **0.**: Zero
- **NG2**: Number of Secondary Positions (always 2)
- **NOR**: Probability Table Order for Current Group
- **NW**: Number of Orders in LIST (NLTP*NG2*NOR)
- **IG**: Group Index for this Record
- **A(NW)**: Data for LIST (NW words), whose content is (PROB(IOR), SIGMA(IOR), IOR=1,NOR)

The last group is always required and is followed by a SEND record. The file ends with a FEND record.
### Figure 4  Sample MERGE Output for U²³⁸ (Room Temperature Only).

<table>
<thead>
<tr>
<th>MATERIAL IDENTIFIER (EA)</th>
<th>- 92238.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MATERIAL IDENTIFIER (MAT)</td>
<td>- 923</td>
</tr>
<tr>
<td>MATERIAL TEMPERATURE</td>
<td>- 293</td>
</tr>
<tr>
<td>NUMBER OF GROUPS</td>
<td>- 1968</td>
</tr>
<tr>
<td>FROM 1.1000E-04 TO 1.9640E+07 EV</td>
<td></td>
</tr>
</tbody>
</table>

#### GROUP STRUCTURE:

<table>
<thead>
<tr>
<th>E b</th>
<th>E f</th>
<th>E b - E f</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9640E+07</td>
<td>1.9477E+07</td>
<td>1.9155E+07</td>
</tr>
<tr>
<td>1.8076E+07</td>
<td>1.7926E+07</td>
<td>1.7624E+07</td>
</tr>
<tr>
<td>1.6625E+07</td>
<td>1.6408E+07</td>
<td>1.6215E+07</td>
</tr>
<tr>
<td>1.5424E+07</td>
<td>1.5206E+07</td>
<td>1.5015E+07</td>
</tr>
<tr>
<td>1.4204E+07</td>
<td>1.3986E+07</td>
<td>1.3795E+07</td>
</tr>
<tr>
<td>1.3084E+07</td>
<td>1.2866E+07</td>
<td>1.2675E+07</td>
</tr>
<tr>
<td>1.1954E+07</td>
<td>1.1736E+07</td>
<td>1.1545E+07</td>
</tr>
<tr>
<td>1.0824E+07</td>
<td>1.0606E+07</td>
<td>1.0414E+07</td>
</tr>
</tbody>
</table>

#### GROUP READ FROM UNIT-19:

<table>
<thead>
<tr>
<th>E b</th>
<th>E f</th>
<th>E b - E f</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000E+10</td>
<td>1.0000E+03</td>
<td>3.0000E+02</td>
</tr>
<tr>
<td>2.0000E+02</td>
<td>5.0000E+02</td>
<td>5.0000E+02</td>
</tr>
<tr>
<td>4.0000E+02</td>
<td>7.0000E+02</td>
<td>7.0000E+02</td>
</tr>
<tr>
<td>1.0000E+01</td>
<td>1.4637E+01</td>
<td>1.4637E+01</td>
</tr>
<tr>
<td>1.6653E+07</td>
<td>1.5835E+07</td>
<td>1.5835E+07</td>
</tr>
<tr>
<td>1.4000E+07</td>
<td>1.3556E+07</td>
<td>1.3556E+07</td>
</tr>
<tr>
<td>1.0000E+01</td>
<td>1.0000E+01</td>
<td>1.0000E+01</td>
</tr>
</tbody>
</table>

#### TEST ON INFINITE DILUTION CROSS SECTIONS:

| MATERIAL VALUE OF BACKGROUND CROSS SECTION IN GENDOF TAPS = 1.0000E+10 (ASSUMED AS INFINITE) |
| COMPARISON ON CROSS SECTION HT= 1 |
| LIST OF DIFFERENCES GREATER THAN 0.0100 |

<table>
<thead>
<tr>
<th>NCOM</th>
<th>SGROUP</th>
<th>EINF</th>
<th>EDSP</th>
<th>SIGMA GENDOF</th>
<th>SIGMA P.T.</th>
<th>DELTA</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>173</td>
<td>6.5900E+00</td>
<td>6.5849E+00</td>
<td>5.22539E+02</td>
<td>5.09119E+02</td>
<td>0.0242</td>
</tr>
<tr>
<td>2</td>
<td>177</td>
<td>6.7514E+00</td>
<td>6.8079E+00</td>
<td>8.11793E+02</td>
<td>8.22051E+02</td>
<td>-0.0125</td>
</tr>
<tr>
<td>3</td>
<td>225</td>
<td>1.0156E+01</td>
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<td>1.06414E+03</td>
<td>1.02861E+03</td>
<td>0.0364</td>
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<tr>
<td>4</td>
<td>226</td>
<td>1.0156E+00</td>
<td>1.0163E+00</td>
<td>1.36822E+02</td>
<td>1.41378E+02</td>
<td>-0.0458</td>
</tr>
<tr>
<td>5</td>
<td>227</td>
<td>1.3268E+01</td>
<td>1.3276E+01</td>
<td>1.57266E+02</td>
<td>1.57270E+02</td>
<td>-0.0004</td>
</tr>
<tr>
<td>6</td>
<td>228</td>
<td>1.0320E+01</td>
<td>1.0413E+01</td>
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<td>1.62243E+01</td>
<td>-0.0015</td>
</tr>
<tr>
<td>7</td>
<td>204</td>
<td>1.9450E+00</td>
<td>1.9676E+00</td>
<td>8.4140E+00</td>
<td>8.3182E+00</td>
<td>0.0018</td>
</tr>
</tbody>
</table>

| 8    | 1053   | 9.9942E+00 | 1.0078E+00 | 1.50971E+02 | 1.79060E+02 | -0.2128 |
| 9    | 1054   | 1.0378E+00 | 1.0382E+00 | 1.54468E+01 | 1.70792E+01 | -0.1444 |
| 10   | 1055   | 1.0162E+00 | 1.0247E+00 | 1.53432E+00 | 1.57275E+00 | -0.0407 |
| 11   | 1056   | 1.0247E+00 | 1.0330E+00 | 1.54175E+00 | 1.57484E+00 | -0.1241 |
| 180  | 1303   | 7.8938E+00 | 7.9500E+00 | 1.24260E+01 | 1.22509E+01 | 0.0141 |
| 181  | 1304   | 9.5500E+00 | 7.9599E+00 | 1.24165E+01 | 1.36229E+01 | -0.0734 |
| 182  | 1305   | 6.2297E+00 | 8.5000E+00 | 1.23670E+01 | 1.29328E+01 | -0.0436 |
| 183  | 1310   | 8.2500E+00 | 8.2986E+00 | 1.33617E+01 | 1.21252E+01 | 0.0195 |

#### SUMMARY:

- 183 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 1.0000E+10 BARGS
- 184 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 1.0000E+03 BARGS
- 177 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 1.0000E+05 BARGS
- 191 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 1.0000E+07 BARGS
- 183 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 2.0000E+01 BARGS
- 192 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 2.0000E+03 BARGS
- 225 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1 AT DILUTION 1.0000E+00 BARGS

**Comparison on Cross Section HT= 2**

<table>
<thead>
<tr>
<th>NCOM</th>
<th>SGROUP</th>
<th>EINF</th>
<th>EDSP</th>
<th>SIGMA GENDOF</th>
<th>SIGMA P.T.</th>
<th>DELTA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**bottom of Resolved (1E-5 eV)**

**top of Resolved (10 KeV)**

**bottom of Unresolved (10 KeV)**

**top of Unresolved (300 KeV)**

**bottom of Resolved (1E-5 eV)**
**Figure 4** Sample MERGE Output for U$^{238}$ (Room Temperature Only). (Continued.)

| 1 | 172 | 6.47593E+00 | 6.53104E+00 | 9.19754E-01 | 9.54616E-01 | -0.0092 | bottom of Resolved (10 KeV) |
| 2 | 173 | 5.53104E+00 | 6.59479E+00 | 1.62324E+00 | 1.43739E+00 | 0.1453 |
| 3 | 308 | 2.01130E+00 | 2.02860E+00 | 1.92730E+00 | 1.97486E+00 | 0.0026 |
| 4 | 375 | 3.31040E+00 | 3.54890E+00 | 9.25882E+00 | 8.78935E+00 | 0.0650 |
| 5 | 449 | 6.53104E+00 | 6.67719E+00 | 7.40572E+00 | 7.32193E+00 | 0.0012 |
| 6 | 575 | 1.86170E+00 | 1.87980E+00 | 7.79067E+00 | 7.47441E+00 | 0.1513 |
| 7 | 1053 | 9.99472E+00 | 1.00798E+00 | 1.43792E+00 | 1.62415E+00 | -0.1201 |
| 8 | 1054 | 1.00798E+00 | 1.01620E+00 | 1.47314E+00 | 1.62742E+00 | -0.0948 |
| 9 | 1055 | 1.01620E+00 | 1.02470E+00 | 1.47190E+00 | 1.48915E+00 | -0.0757 |
| 10 | 1056 | 1.02470E+00 | 1.03330E+00 | 1.47065E+00 | 1.28379E+00 | 0.1456 |

**top of Resolved (10 KeV)**

| 185 | 1303 | 7.89389E+00 | 7.85000E+00 | 1.10226E+00 | 1.18633E+00 | 0.0145 |
| 26 | 1304 | 7.95000E+00 | 7.85900E+00 | 1.10161E+00 | 1.27547E+00 | -0.0745 |
| 27 | 1309 | 8.22950E+00 | 0.25030E+00 | 1.17450E+00 | 1.25585E+00 | -0.0419 |
| 28 | 1310 | 8.25000E+00 | 0.39810E+00 | 1.17367E+00 | 1.35214E+00 | 0.0187 |

**bottom of Unresolved (300 KeV)**

### SUMMARY:
- **180** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 1.000E+00 BANKS
- **160** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 2.000E+00 BANKS
- **140** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 3.000E+00 BANKS
- **120** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 4.000E+00 BANKS
- **100** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 5.000E+00 BANKS
- **80** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 6.000E+00 BANKS
- **60** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 7.000E+00 BANKS
- **40** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 8.000E+00 BANKS
- **20** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 9.000E+00 BANKS
- **10** DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 2 AT DILUTION 1.000E+01 BANKS

### COMPARISON ON CROSS SECTION NT+ 4

**LIST OF DIFFERENCES GREATER THAN 0.0100**

<table>
<thead>
<tr>
<th>WDN</th>
<th>NGROUP</th>
<th>EINF</th>
<th>ESUP</th>
<th>SIGMA GENDF</th>
<th>SIGMA P.T.</th>
<th>DELTA</th>
</tr>
</thead>
<tbody>
<tr>
<td>29</td>
<td>1235</td>
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<td>4.51650E+00</td>
<td>9.65569E-05</td>
<td>1.08391E-03</td>
<td>-0.0094</td>
</tr>
<tr>
<td>30</td>
<td>1236</td>
<td>4.51650E+00</td>
<td>4.55480E+00</td>
<td>3.42687E-03</td>
<td>1.55741E-03</td>
<td>1.2004</td>
</tr>
<tr>
<td>31</td>
<td>1237</td>
<td>4.55480E+00</td>
<td>4.59249E+00</td>
<td>8.35241E-03</td>
<td>9.56715E-03</td>
<td>-0.1249</td>
</tr>
<tr>
<td>32</td>
<td>1238</td>
<td>4.59249E+00</td>
<td>4.63022E+00</td>
<td>1.33236E-02</td>
<td>1.21475E-02</td>
<td>0.0968</td>
</tr>
</tbody>
</table>

**bottom of Unresolved (10 KeV)**

| 33 | 1303 | 7.89389E+00 | 7.95000E+00 | 3.93158E-01 | 3.85893E-01 | 0.0187 |
| 34 | 1304 | 7.95000E+00 | 7.95940E+00 | 1.14662E+00 | 1.12627E+00 | 0.0014 |
| 35 | 1305 | 7.95940E+00 | 7.99500E+00 | 1.04592E+00 | 1.04499E+00 | 0.0016 |
| 36 | 1306 | 7.99500E+00 | 8.03960E+00 | 1.05406E+00 | 1.03584E+00 | 0.0078 |
| 37 | 1307 | 8.03960E+00 | 8.08390E+00 | 1.02123E+00 | 1.01185E+00 | 0.0079 |
| 38 | 1308 | 8.08390E+00 | 8.12500E+00 | 1.00082E+00 | 9.88847E+01 | 0.0195 |
| 39 | 1309 | 8.12500E+00 | 8.16250E+00 | 8.85128E+01 | 9.70565E+01 | 0.0160 |

**SUMMARY:** 39 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 4 AT DILUTION 1.000E+00 BANKS

### COMPARISON ON CROSS SECTION NT+ 10

**LIST OF DIFFERENCES GREATER THAN 0.0100**

<table>
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<th>WDN</th>
<th>NGROUP</th>
<th>EINF</th>
<th>ESUP</th>
<th>SIGMA GENDF</th>
<th>SIGMA P.T.</th>
<th>DELTA</th>
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<td>9.14907E-06</td>
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</tbody>
</table>

**bottom of Resolved (1E-5 eV)**

-- all differences < 3%

**top of Resolved (10 KeV)**

**bottom of Unresolved (10 KeV)**
**Figure 4** Sample Merge Output for U^{238} (Room Temperature Only). (Continued)

| 187 | 1504 | 4.0722E+05 | 4.1103E+05 | 2.6217E+04 | 2.6586E+04 | -0.018 |
| 188 | 1500 | 4.1230E+05 | 4.1447E+05 | 2.6618E+04 | 2.7026E+04 | -0.024 |
| 189 | 1525 | 4.8557E+05 | 4.8941E+05 | 3.6435E+04 | 3.4217E+04 | -0.121 |
| 190 | 1527 | 4.8537E+05 | 4.8537E+05 | 3.6524E+04 | 3.5140E+04 | -0.151 |
| 191 | 1527 | 4.9373E+05 | 4.8711E+05 | 3.6621E+04 | 3.2949E+04 | -0.151 |
| 192 | 1501 | 6.0305E+05 | 6.0019E+05 | 8.5180E+03 | 8.3793E+03 | -0.147 |
| 193 | 1552 | 6.0010E+05 | 6.1318E+05 | 8.7858E+03 | 8.5798E+03 | -0.025 |
| 194 | 1552 | 6.1320E+05 | 6.1832E+05 | 9.0527E+03 | 8.8889E+03 | -0.025 |
| 195 | 1556 | 6.2087E+05 | 6.3993E+05 | 9.0739E+03 | 1.1922E+03 | -0.012 |
| 196 | 1570 | 7.0542E+05 | 7.1434E+05 | 1.8791E+03 | 1.8597E+03 | -0.019 |
| 197 | 1602 | 7.8002E+05 | 7.8416E+05 | 1.7440E+03 | 1.7432E+03 | -0.008 |
| 198 | 1593 | 8.5975E+05 | 8.6938E+05 | 8.2902E+03 | 8.0487E+03 | -0.020 |
| 199 | 1591 | 9.3175E+05 | 9.7035E+05 | 9.0479E+03 | 8.9780E+03 | -0.035 |
| 200 | 1595 | 8.7015E+05 | 8.7743E+05 | 1.0024E+03 | 9.8681E+03 | -0.018 |

**SUMMARY:** 260 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 1.000E+03 BANKS

**SUMMARY:** 199 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 1.000E+03 BANKS

**SUMMARY:** 200 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 3.000E+02 BANKS

**SUMMARY:** 198 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 5.000E+01 BANKS

**SUMMARY:** 260 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 1.000E+04 BANKS

**SUMMARY:** 261 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 1B AT DILUTION 1.000E+04 BANKS

**COMPARISON ON CROSS SECTION HT-101**

**LIST OF DIFFERENCE GREATER THAN 0.0100**

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<th>SIGMA</th>
<th>SIGMA</th>
<th>SIGMA</th>
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<td>1.7282E+00</td>
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<td>9.0000E-02</td>
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</tr>
</tbody>
</table>

**Bottom of Resolved (1E-5 eV)**

46
Figure 4  Sample MERGE Output for U^{238} (Room Temperature Only). (Continued)

| 352 | 1802 | 4.08378E+06 | 4.9764E+06 | 2.32304E-03 | 2.32078E-03 | 0.0105  |
| 353 | 1853 | 4.9264E+06 | 4.9605E+06 | 2.22467E-03 | 2.19644E-03 | 0.0128  |
| 354 | 1806 | 5.04931E+06 | 5.0516E+06 | 2.01486E-03 | 1.99448E-03 | 0.0103  |
| 355 | 1807 | 5.9316E+06 | 5.13417E+06 | 1.97847E-03 | 1.97766E-03 | 0.0105  |

SUMMARY: 355 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+10 BARNs

SUMMARY: 358 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+03 BARNs

SUMMARY: 359 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+02 BARNs

SUMMARY: 355 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 5.0000+01 BARNs

SUMMARY: 407 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 2.0000+01 BARNs

SUMMARY: 404 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+01 BARNs

SUMMARY: 534 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+00 BARNs

COMPARISON ON CROSS SECTION MT= 15

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<th>NCON</th>
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<th>ESUP</th>
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<th>SIGMA P.T.</th>
<th>DELTA</th>
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SUMMARY: 18 DIFFERENCES GREATER THAN 0.0100 IN CROSS SECTION 101 AT DILUTION 1.0000+10 BARNs

********** CORRECTIVE FACTORS FOR SCATTERING MATRICES **********

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<th>NDSUP</th>
<th>INF</th>
<th>ESUP</th>
<th>CORR. ELAST</th>
<th>CORR. INCL.</th>
<th>CORR. FISS.</th>
<th>CORR. CAPT.</th>
<th>CORR. N,VE</th>
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<td>9.99999E-01</td>
<td>1.00000E+00</td>
<td>1.00000E+00</td>
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</table>

1968 1.94773E+07 1.96493E+07 9.99957E-01 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00027E+00

48
Summation Checks

1) ECCO Primaries

\[ \text{TOTAL} = \text{ELASTIC} + \text{INELASTIC} + (n,Mn) + \text{FISSION} + \text{CAPTURE} \]

2) INELASTIC Components

Cross-section for the production of one neutron in an exit channel

\[ \text{MT4} = \sum_{n=51}^{91} \text{MTn} \]

3) FISSION

\[ \text{TOTAL FISSION} = \text{Sum of first, second, third and fourth chance fission} \]

\[ \text{MT18} = \text{MT19} + \text{MT20} + \text{MT21} + \text{MT38} \]
Matrix Rows Sum to Primaries

1) ELASTIC

\[ \sigma_{el}^G = \sum_{G'} \sigma_{el}^{G-G'} \]

MF3, MT2 = MF6, MT2
MF3, MThERM = MF6, MThERM (overrides where present)

2) INELASTIC

\[ \sigma_{inel}^G = \sum_C \sum_{G'} \sigma_C^{G-G'} \]

Components (C) are:
- INELASTIC levels: MT 51 - 90
- INELASTIC continuum: MT 91
- \((n, n' + \alpha)\): MT 22
- \((n, n' + 3\alpha)\): MT 23
- \((n, n' + p)\): MT 28
- \((n, n' + 2\alpha)\): MT 29
- \((n, n' + d)\): MT 32
- \((n, n' + t)\): MT 33
- \((n, n' + He^3)\): MT 34
- \((n, n' + d + 2\alpha)\): MT 35
- \((n, n' + t + 2\alpha)\): MT 36

3) \((n, Mn)\)

\[ \sigma_{(n, Mn)}^G = \sum_{M=1}^{4} \sum_{G'} \frac{1}{M} \sigma_{(n, Mn)}^{G-G'} P \]

\(M\) indicates the number of neutrons produced
\(P\) indicates additional products (i.e. blank, \(\alpha\), \(p\))
Resonance Self Shielding

Compare the infinite dilution cross-section for the Primary formed from MF = 3 data with that formed from MF = 50 data:

\[ \sigma^G_{\text{Primary}} = \sum_{g \in G} P^G g \sigma^G_{\text{Primary}} \]

where

- \( G \) indicates energy group
- \( g \) indicates sub group

Primaries are TOTAL, ELASTIC, CAPTURE, (FISSION and INELASTIC)\(^*\)

\(^*\) check yet to be included.

Additional

Fission Spectra

\[ \sum_{G'} \chi^G_{F'} = 1.0 \]

\( \chi^G_{F'} \) is the average nuclide dependant total fission spectrum.

Averaged over incident groups:

\[ \bar{\chi}^G_{F'} = \frac{\sum_G (\chi^G_{F} \sigma^G_{F} \chi^G_{G'}) \phi^G}{\sum_G (\chi^G_{F} \gamma^G_{G'}) \phi^G} \]

\[ \bar{\chi}^G_{F'} = \frac{\sum_G (\text{MF6, MT18}) \phi^G}{\sum_G (\text{MF3, MT18}) \phi^G} \]

in the absence of delayed neutrons.

\( \phi^G \) should be supplied to CRECCO (fast Reactor Flux).

Full formulae are available in Reference 19.

Mean Scattering Angle

\[ \bar{\mu}_G = \frac{\sum (\sigma^G_{e} \rightarrow G')}{\sigma^G_{e}} \]

\[ \sum (\text{MF6, MT2 or MF6, MOTHERM}) \]

\[ \text{MF3, MT251} = \frac{\sum (\text{MF3, MT2 or MF3, MOTHERM})}{\text{MF3, MT2 or MF3, MOTHERM}} \]

MOTHERM overrides where present.
Table 1  Formation of “CALENDF reactions” from the Components on the GENDF

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<th>Reactions Compared from GENDF</th>
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<tr>
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<td>PARASITIC ABSORPTION</td>
<td>101, 102-109, 111-116</td>
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<td>Reaction Name</td>
</tr>
<tr>
<td>------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>1</td>
<td>TOTAL</td>
</tr>
<tr>
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<td>ELASTIC</td>
</tr>
<tr>
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<td>TOTAL NONELASTIC</td>
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<td>TOTAL INELASTIC</td>
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<td>n, 3n + f</td>
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<tr>
<td>39 - 40</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>n, 2n + p</td>
</tr>
<tr>
<td>42</td>
<td>n, 3n + p</td>
</tr>
<tr>
<td>43-49</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td></td>
</tr>
<tr>
<td>51-91</td>
<td>INELASTIC LEVELS and CONTINUUM</td>
</tr>
<tr>
<td>92-100</td>
<td></td>
</tr>
<tr>
<td>101</td>
<td>TOTAL_CAPTURE</td>
</tr>
<tr>
<td>102</td>
<td>n, γ</td>
</tr>
<tr>
<td>103</td>
<td>n, p</td>
</tr>
<tr>
<td>104</td>
<td>n, d</td>
</tr>
<tr>
<td>105</td>
<td>n, t</td>
</tr>
<tr>
<td>106</td>
<td>n, He³</td>
</tr>
<tr>
<td>107</td>
<td>n, α</td>
</tr>
<tr>
<td>108</td>
<td>n, 2α</td>
</tr>
<tr>
<td>109</td>
<td>n, 3α</td>
</tr>
<tr>
<td>110</td>
<td></td>
</tr>
<tr>
<td>111</td>
<td>n, 2p</td>
</tr>
<tr>
<td>112</td>
<td>n, p + α</td>
</tr>
<tr>
<td>113</td>
<td>n, t + 2α</td>
</tr>
<tr>
<td>114</td>
<td>n, d + 2α</td>
</tr>
<tr>
<td>115</td>
<td>n, p + d</td>
</tr>
<tr>
<td>116</td>
<td>n, p + t</td>
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<tr>
<td>117-200</td>
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</tr>
<tr>
<td>201-250</td>
<td></td>
</tr>
<tr>
<td>&gt;250</td>
<td></td>
</tr>
</tbody>
</table>

* Improvements required
Session 2:

SPECIFIC PRESENTATIONS: ADDITIONAL MODULES, ASPECTS OF PROCESSING REQUIRING FURTHER ATTENTION

Chair:
Cheikh Diop, Christopher Dean,
and Caroline Raepsaet
INTERPOLATION IN THE UNRESOLVED RESONANCE REGION

John L. ROWLANDS

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ABSTRACT

Comparisons between NJOY/THEMIS and CAENDF have indicated significant differences in the unresolved resonance region for several isotopes in JEF-2. The problem is one of interpolation. In NJOY the interpolation is linear in energy between the cross-section values calculated at the points where the resonance parameters are tabulated, or at the ends of the range if there is a single set of parameters for the unresolved region. This is not a satisfactory method when the points are well separated or when the range having a single set of parameters is large.
Comparisons made between NJOY/UNRESR/GROUPR calculations and CAENDF (resonance ladder) calculations for the unresolved resonance range have shown some large differences (e.g. factor of 5) which result from the methods of interpolation.

The method used in NJOY-89 is to calculate cross-section values only at the energies at which parameters are specified (or at the ends of the ranges for which they are specified) and to use linear x linear interpolation to obtain values at intermediate energies. When the range is wide this can produce values which are substantially different from the cross-section values obtained using the average parameters at the intermediate points, as is done in CAENDF.

By way of illustration, consider the case of Cm-245 for which there is a single unresolved range, from 61 eV to 10 keV, in which the average parameters are constant.

Resonant component of the total cross-section

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>UNRESR and interpolation</th>
<th>Calculated from parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>61</td>
<td>62.9</td>
<td>62.9</td>
</tr>
<tr>
<td>100</td>
<td>62.6</td>
<td>49.1</td>
</tr>
<tr>
<td>300</td>
<td>61.5</td>
<td>28.4</td>
</tr>
<tr>
<td>1000</td>
<td>57.4</td>
<td>15.5</td>
</tr>
<tr>
<td>3000</td>
<td>45.9</td>
<td>9.2</td>
</tr>
<tr>
<td>10000</td>
<td>5.4</td>
<td>5.4</td>
</tr>
</tbody>
</table>

The use, here, of a single energy range, from E to 164E, is clearly unsatisfactory with the present NJOY-89 interpolation method.

Referring to the Data Formats and Procedures Guide, ENDF-102 (July, 1990), the recommendations given in section 2.42. "Interpolation in the Unresolved Resonance Region (URR)" are:

a) For energy dependent formats:

(i) Interpolate on the cross-sections derived from the parameters.

(ii) If two adjacent grid points differ in energy by more than a factor of three the processing code should add intermediate points (with a spacing of about 10 per decade) and compute the values at these points using parameter interpolation.

b) When a single set of parameters is given for the unresolved range:

(ii) The processing code should generate a set of intermediate energies (approximately 10 per decade) and compute the cross-sections at these points using the parameters.
Nevertheless it would be safer if evaluations were to have tabulations at a sufficient number of energy points to give the required accuracy using linear interpolation in the cross-sections calculated from the parameters at the tabular points.

To give an indication of the number of energy points which must be used in the tabulation consider a cross-section which varies as \(1/E\), \(\sigma(E) = C/E\), and an energy range from \(E_1\) to \(E_2 = R \cdot E_1\); that is 
\[
\sigma_1 = C/E_1; \quad \sigma_2 = C/E_2 = \frac{\sigma_1}{R^{1/2}}
\]

Consider the average value over the range \(E_1\) to \(E_2\)
\[
I = \int_{E_1}^{E_2} \sigma(E) \, dE / \int_{E_1}^{E_2} dE = 2\sigma_1/(1 + R^{1/2})
\]

Now consider the value obtained using linear interpolation between \(\sigma_1\) and \(\sigma_2\)
\[
\sigma'(E) = \frac{\sigma_1 E_2 - \sigma_2 E_1}{(E_2 - E_1)} + \frac{(\sigma_2 - \sigma_1)}{(E_2 - E_1)} E
\]
\[
= \frac{\sigma_1 (R^{3/2} - 1)}{R^{1/2} (R-1)} - \frac{\sigma_1}{E_1} \left( \frac{R^{1/2} - 1}{R^{1/2} (R-1)} \right) E
\]

Integrating we obtain:
\[
I' = \sigma_1 (R^{1/2} + 1) / 2R^{1/2}
\]
and so the ratio is
\[
I'/I = (R^{1/2} + 1)^2 / 4 R^{1/2}
\]

When \(R = 2\), \(I'/I = 1.03\)
and the average value of the cross-section is overestimated by 3%.

For a 1% accuracy we must have an energy spacing of a factor of 1.5 or less.

A better procedure is to specify the infinite dilute cross-section values, then the error will only be in the shielding factors at intermediate values of the energy and the variations in this are smaller. However, the infinite dilution cross-sections must be specified on a fine energy mesh, and the mean parameters should not be on a widely spaced mesh.
APPROXIMATIONS IN THE TREATMENT OF DOPPLER BROADENING:
SECONDARY ENERGY DISTRIBUTIONS AND SOLID STATE EFFECTS

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ABSTRACT

Doppler broadening calculations are made in NJOY using the monatomic gas model (or Maxwellian velocity distribution). This is expected to be satisfactory for high temperatures and high neutron energies, but it might not be satisfactory for resonances below about 10 eV at ambient temperature.

The effects of Doppler broadening on secondary energy distributions are neglected at the present time (except in the thermal energy range). Recent studies have shown these effects to be significant, and the distributions to vary markedly through the resonances of $^{238}$U.
There are two aspects of the calculation of Doppler broadening which are not treated at present in NJOY, nor, for that matter, in any reactor physics calculational scheme. This brief paper is written to note these aspects because it is thought that, in some cases, they might not be negligible: one effect is the influence of solid state thermal motion on Doppler broadening. At present only the monatomic gas model is available in NJOY for calculating Doppler broadening. The thermal scattering treatment only applies to constant scattering cross-sections. The other effect is the influence of the thermal motion on secondary energy distributions of neutrons scattered in resonances. At present this effect is neglected, the secondary energy distribution being assumed to be that of a nucleus initially at rest. Again this effect cannot be treated at present because of the assumption of constant cross-sections in the thermal scattering treatment.

At high energies and high temperatures solid state effects can be treated using the gas model with an effective temperature. However, for energies below about 10 eV and at temperatures of about 300 K (or lower) the use of the gas model with an effective temperature is not so accurate, for example for U in UO₂. The broadening is not as much as that given by the gas model with an effective temperature and the shape is modified. The Doppler broadened capture cross-section line shape has been calculated for the 6.7 eV resonance in ²³⁸U (see Borgonovi et al., 1969 (1)) using the weighted phonon frequency spectrum for U in UO₂ included in the ENDF/B thermal scattering data. The result is reproduced in Fig. 1 and we see that the peak height is closer to the gas model value calculated for the actual temperature of 296 K, rather than for the effective temperature (calculated from the mean kinetic energy), which is 311.1 K (the equivalent Debye temperature is 300 K). We can also see that the peak energy is moved, slightly, to a lower energy, and there is a small change in the symmetry of the resonance.

At lower energies the measurements made by Liou and Chrion (1981) (2) of the capture cross-section in the 1 eV resonance of ²⁴⁰Pu, (for Pu in PuO₂), show that the Doppler broadening can be less than that calculated using the gas model for the actual temperature (Fig. 2). For measurements made at 296 K the analysis of the shape made using the gas model gave a best fit with an effective temperature of 277 ± 9 K. The value of $\chi^2$/degree was 1.412 suggesting that the shape was not well represented by gas model Doppler broadening.

The way the shape differs from the gas model broadened shape is illustrated by calculations made by Seidel et al. (1989) (3) for the 6.7 eV resonance in ²³⁸U for U in UO₂. They use a simpler model for the weighted phonon frequency spectrum than that in ENDF/B, a simple, two frequency, Nernst-Lindemann model:

$$\rho(\varepsilon) = a_1 \delta(\varepsilon - \varepsilon_1) + a_2 \delta(\varepsilon - \varepsilon_2)$$

the energies corresponding to the two basic frequencies being

$$\varepsilon_1 = 12 \pm 3 \text{ meV} \text{ and } \varepsilon_2 = 46 \pm 4 \text{ meV}$$
and the coefficients are

\[ a_1 = 0.92 \pm 0.02 \text{ and } a_2 = (1-a_1) \]

The equivalent Debye temperature is 260°K.

The way the calculated shapes differ from the gas model values is illustrated in Fig. 3.

A question which has not been considered is whether the shape of the scattering cross-section is changed in the same way as the capture cross-section. Shamaoun and Summerfield (1990) (4) and Kuwaffi and Summerfield (1991) (5) have shown that in the high energy or high temperature limits, (when Lamb's approximation applies and an effective temperature can be used in the gas model to calculate the broadening) the effective temperature to be used in calculating the broadening of the scattering cross-section is the same as that used to calculate the broadening of the capture cross-section. If the broadened shapes are the same for the capture and scattering cross-sections then probably the small change in the shape of the Doppler broadened resonance (relative to the gas model broadened shape) is of minor importance and it is only the effective temperature to be used in calculating the broadening which needs to be considered. This could be energy dependent at low neutron energies.

The methods for calculating Doppler broadened capture cross-section line shapes from the weighted phonon frequency distribution have been described by Jackson and Lynn (1962) (6), and by Borgonovi et al (1969), and the methods of Shamaoun and Summerfield can be developed to calculate the broadening of the scattering cross-section.

A recent study by Ouisloumen and Sanchez (1991) (7) has shown how large the effect of thermal motion is on the energy distribution of neutrons scattered by heavy nuclei up to energies of about 100 eV and how strongly these distributions vary though \(^{238}\text{U}\) resonances. The study used the monatomic gas model. The secondary distributions are significantly broadened and the mean energy of the scattered neutrons is moved towards the energy of the resonance peak (in c.m. coordinates) for neutrons scattered within the energy range of the broadened resonance. The fraction of the neutrons scattered up in energy can be large for neutrons scattered at energies below the peak of the resonance. The results of the calculations made by Ouisloumen and Sanchez are reproduced in Figs. 4 and 5. These are for the resonances at 6.7 eV and for a temperature of 1000°K. The upscattering probability for the energy point below the peak of the 6.7 eV resonance is 82% and below the peak of the 36.7 eV resonance it is 54%.

The formulae for the secondary energy distribution \((P_0 \text{ and } P_1 \text{, components})\) involve integrals of a temperature dependent function and the unbroaded cross-section (see, for example, Blackshaw and Murray, 1967). One could envisage calculating the scattering matrix (for \(^{238}\text{U}\), for example) in a fine group structure. The flux calculation would be more complicated than in the methods currently used because of upscattering being present.

63
REFERENCES

Figure 1: Doppler broadened line shape for 6.67 eV resonance of $^{238}\text{U}$ at $T = 296^\circ\text{K}$

(From Bourgonovi et al)
Figure 2: An example of the shape fit, for the effective temperature $T'$, to $^{240}$Pu oxide capture data measured at room temperature. $\Gamma_n = 2.32$ meV and $\Gamma_y = 32.7$ meV are assumed. The results are $T' = 277 \pm 9^\circ$K and $\chi^2$/degree $= 1.412$ (From Liou and Chrien)
Figure 3: Difference $\Delta \sigma$ and ratio $\sigma/\sigma_0$ for 6.67 eV resonance cross-sections for $^{238}$U calculated for vibrations in the lattice and using the gas model for values of $T = 300$ and $600$ K.

(From Seidel et al)
Figure 4: Effective transfer kernel of $^{238}\text{U}$ at 1000 K near the 6.67 eV resonance for neutrons of energy (a) 6.52 eV and (b) 7.2 eV. The corresponding upscattering probabilities are 82.03 and 28.12%, respectively. (From Guilloumen and Sanchez)

Figure 5: Effective transfer kernel of $^{238}\text{U}$ at 1000 K near the 36.67 eV resonance for neutrons of energy (a) 36.25 eV and (b) 37.2 eV. The corresponding upscattering probabilities are 54.23 and 7.95%, respectively. (From Guilloumen and Sanchez)
TRANSX TODAY AND TOMORROW*

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Los Alamos, New Mexico 87545

ABSTRACT

TRANSX 2.0 is the latest release in the TRANSX series. These codes are used to prepare cross-section tables for use in a variety of nuclear transport calculations. This version has been modernized and cleaned up, but its capabilities are basically the same as for the earlier releases. The next few versions will add significant new capabilities, such as detailed multi-region flux calculations, which will make TRANSX much more useful for complex problems.

I. INTRODUCTION

Many problems in nuclear technology require detailed calculations of the distribution in space and energy of neutrons, photons, and other particles. These calculations are normally made with discrete-ordinates codes like ONEDANT,\textsuperscript{1} TWODANT,\textsuperscript{2} or ANISN,\textsuperscript{3} with diffusion codes like DIF3D,\textsuperscript{4} or even with Monte-Carlo codes with a multigroup capability like MCNP.\textsuperscript{5} All of these codes require cross-section data in the form of a "transport table." The TRANSX series of codes\textsuperscript{6,7} was developed to allow users to prepare transport tables from up-to-date nuclear libraries in MATXS format prepared with the NJOY nuclear data processing system.\textsuperscript{8,9,10,11} Some of the key features of TRANSX follow.

- Neutron tables, photon tables, or coupled sets, including charged particles.
- Material or groupwise ordering in direct or adjoint form.
- Mixtures for use as macroscopic cross sections or for making elements from isotopes.
- Collapsing to a subset group structure.
- Spatial collapse to compute cell-average cross sections.

---

• Self-shielding for homogeneous and simple heterogeneous systems, including simple Dancoff corrections.

• Thermal upscatter cross sections.

• A variety of transport corrections is available.

• Response function edits that are any linear combination of the library cross sections, including heating and damage.

• Several commonly used output formats.

• Easily transportable between different computer systems.

These features will be illustrated by a series of examples in the subsequent sections of this report.

Although this version of TRANSX is useful for a wide variety of nuclear problems, it is weak in its treatment of resonance self-shielding for thermal-reactor problems. This report will conclude with a preview of the methods that will be used to remove this deficiency in future versions of TRANSX.

II. SIMPLE TRANSPORT TABLES

The use of TRANSX to produce some very simple transport tables is illustrated by the following input deck. The general idea is to produce $P_0$ and $P_1$ tables for three materials. One of them is a combination of four isotopes to produce elemental tungsten.

```
SIMPLE MATERIAL ORDERED TABLES
0 1 0 1 1 1 0 3 0 0
30 2 33 0 0 3 1 6 0 0
CARBON TUNGST U-235
* */
1 1 CNAT/
2 1 W182 .263/
2 1 W183 .143/
2 1 W184 .307/
2 1 W186 .286/
3 1 U235/
STOP
```

The meaning of these input parameters and the tables produced by this run are illustrated by the following excerpts from the TRANSX output listing for this input deck.
TRANSPORT CROSS SECTIONS
FROM MATIS LIBRARIES

VERS. 2.0 (6 MAR 92)
RUN ON 3/5/92
AT 15:59:48

---

TITLE

TEST 1 -- MATERIAL ORDERED TABLES

OPTIONS

IPRINT 0 (0=LONG/1=SHORT)
IOUT 1 (0=None/1=CARD/2=CLAW/3=FIDD/4=ANISE/5=GOXS/6=ISOTXS)
IPROB 0 (0=DIRECT/1=ADJOINT)
ISET 1 (1=MM/2=GG/3=COUPLLED)
IFORM 1 (1=MATWISE/2=GROUPWISE)
ITIME 1 (1=STADY-STATE/2=PROMPT)
IDECAY 0 ((RESERVED)
ITRC 3 (0=NO TRANSPORT CORR/1=CONS.P/2=DIGA/3=B-H-S/4=INFLOW)
ICOLL 0 (0=NO COLLAPSE/1=FINE-COLLAPSE)
INITF 0 (0=LIBRARY FLUX/1=FO CARDS/2=RTFLUX/3=RZMFLX/REG FOR ESC)

PARAMETERS

NGROUP 30 GROUPS
NL 2 TABLES
Ntabl 34 POSITIONS IN TABLE
NUP 0 UP SCATTER GROUPS
NTHG 0 NUMBER OF THERMAL GROUPS
NMIX 3 MIXES OR MATERIALS
NREG 1 REGIONS
NMIXS 6 MIXTURE SPECIFICATIONS
NED 0 EXTRA EDIT POSITIONS
NEDS 0 EDIT SPECIFICATIONS

MIX NAMES

1 CARBON
2 TUNGST
3 U-235

REGION TEMP(K) SIZE HETEROGENEITY

1 3.000E+02 1.000E+00 0

SPEC MIX REG NUCLIDE DENSITY THERMAL MATRIX MOD

1 1 1 CNAT 1.000E+00
2 2 1 W182 2.63E-01
3 2 1 W183 1.430E-01
4 2 1 W184 3.070E-01
5 2 1 W186 2.860E-01
6 3 1 U235 1.000E+00

71
INPUT MATXS FILE

FILE ID  MATXS T2LANLJUY  VERS 10
30X12 LIBRARY FROM ENDF/B-VI, JAN 1992

MATERIAL-ORDERED CROSS SECTION TABLES

WORDS AVAILABLE FOR TABLE = 6120
NUMBER OF OUTPUT MIXTURES PER PASS = 3
NUMBER OF LEGENDRE ORDERS PER PASS = 2

FINE FLUX FOR REGION 1  SUM  3.4360E+07
3.723E+03  7.392E+04  1.905E+04  1.410E+04  2.312E+04  4.396E+04 ...

** CARBON PO **

<table>
<thead>
<tr>
<th>POSITION</th>
<th>GROUP 1</th>
<th>GROUP 2</th>
<th>GROUP 3</th>
<th>GROUP 4</th>
<th>GROUP 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 INGRP</td>
<td>5.052E-02</td>
<td>5.846E-02</td>
<td>1.131E-01</td>
<td>1.263E-01</td>
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</tr>
<tr>
<td>5</td>
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</tr>
<tr>
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</tr>
<tr>
<td>7</td>
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<td>0.000E+00</td>
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<td>1.264E-01</td>
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<tr>
<td>8</td>
<td>0.000E+00</td>
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<td>0.000E+00</td>
<td>0.000E+00</td>
<td>5.053E-02</td>
</tr>
</tbody>
</table>

** CARBON P1 ** ...
** TUNGST PO ** ...
** TUNGST P1 ** ...
** U-235 PO ** ...

<table>
<thead>
<tr>
<th>POSITION</th>
<th>GROUP 1</th>
<th>GROUP 2</th>
<th>GROUP 3</th>
<th>GROUP 4</th>
<th>GROUP 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 ABS</td>
<td>1.396E+00</td>
<td>1.468E+00</td>
<td>1.193E+00</td>
<td>9.069E-01</td>
<td>1.160E+00</td>
</tr>
<tr>
<td>2 NUSIGF</td>
<td>9.695E+00</td>
<td>9.046E+00</td>
<td>7.977E+00</td>
<td>6.866E+00</td>
<td>6.445E+00</td>
</tr>
<tr>
<td>3 TOTAL</td>
<td>3.536E+00</td>
<td>3.654E+00</td>
<td>3.719E+00</td>
<td>3.832E+00</td>
<td>3.971E+00</td>
</tr>
<tr>
<td>5</td>
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<td>9.061E-02</td>
<td>1.120E-01</td>
</tr>
<tr>
<td>6</td>
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<td>0.000E+00</td>
<td>3.121E-02</td>
<td>4.763E-02</td>
<td>7.778E-02</td>
</tr>
<tr>
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<td>6.969E-02</td>
</tr>
<tr>
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<td>0.000E+00</td>
<td>0.000E+00</td>
<td>4.663E-02</td>
</tr>
</tbody>
</table>

** U-235 P1 ** ...

TRANSX COMPLETE  2.7S

The definition of some of these parameters and the arrangement of data in a transport table are summarized in Table 1. Note that the scattering matrix in each of these tables is triangular. The group numbering is from high energy
to low energy. Therefore, position 5 for group 2 in the carbon table gives the scattering into group 2 (13.5 to 15 MeV) from group 1 (15 to 17 MeV). Also note that the fission neutron production cross section \textit{NUSIGF} only appears for the fissionable nucleus $^{235}$U.

The transport tables generated by \textsc{TRANSX} can be written out in a variety of formats. The simplest of these is the \textsc{CARD} option using "6E12" cards; this format was used in the pioneering discrete-ordinates transport code \textsc{DTF}. An example of the output for this sample problem follows:

<table>
<thead>
<tr>
<th>CARBON P0</th>
<th>34X 30 TABLE</th>
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</thead>
<tbody>
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<td>0</td>
</tr>
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<td>1</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>2</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>3</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>4</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>5</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>6</td>
</tr>
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<td>6.80773E-01 5.84586E-02 2.61000E-01 0.00000E+00 0.00000E+00 0.00000E+00</td>
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<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>8</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>9</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>10</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>11</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>12</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>13</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>14</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>15</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CARBON P1</th>
<th>34X 30 TABLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00000E+00 0.00000E+00 3.06988E-03 0.00000E+00 4.94349E+00 4.94042E+00</td>
<td>165</td>
</tr>
<tr>
<td>7.53279E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>166</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>167</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>168</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>169</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>170</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>U-235 P0</th>
<th>34X 30 TABLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.39646E+00 9.69490E+00 3.53555E+00 7.10089E-01 0.00000E+00 0.00000E+00</td>
<td>1</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>2</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>3</td>
</tr>
<tr>
<td>0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</td>
<td>4</td>
</tr>
<tr>
<td>Position</td>
<td>Contents for Group $g$</td>
</tr>
<tr>
<td>----------</td>
<td>------------------------</td>
</tr>
<tr>
<td>1</td>
<td>$\sigma_{Eg}$ Response edits</td>
</tr>
<tr>
<td>:</td>
<td>}</td>
</tr>
<tr>
<td>NED</td>
<td></td>
</tr>
<tr>
<td>...........</td>
<td>...........</td>
</tr>
<tr>
<td>NED+1</td>
<td>$\sigma_{eg}$</td>
</tr>
<tr>
<td>NED+2</td>
<td>$\bar{v}<em>g\sigma</em>{fg}$ Standard edits</td>
</tr>
<tr>
<td>NED+3</td>
<td>$\sigma_g$</td>
</tr>
<tr>
<td>...........</td>
<td>...........</td>
</tr>
<tr>
<td>NED+4</td>
<td>...........</td>
</tr>
<tr>
<td>:</td>
<td>}</td>
</tr>
<tr>
<td>NED+NUP+3</td>
<td>$\sigma_{g\rightarrow g'}$ Upscatter ($g' &gt; g$)</td>
</tr>
<tr>
<td>...........</td>
<td>...........</td>
</tr>
<tr>
<td>NED+NUP+4</td>
<td>$\sigma_{g\rightarrow g'}$ In-group ($g' = g$)</td>
</tr>
<tr>
<td>...........</td>
<td>...........</td>
</tr>
<tr>
<td>NED+NUP+5</td>
<td>...........</td>
</tr>
<tr>
<td>:</td>
<td>}</td>
</tr>
<tr>
<td>NED+NUP+5</td>
<td>$\sigma_{g\rightarrow g'}$ Downscatter ($g' &lt; g$)</td>
</tr>
<tr>
<td>...........</td>
<td>...........</td>
</tr>
<tr>
<td>NED=NUP+3</td>
<td>NTABL</td>
</tr>
</tbody>
</table>

**NED** = number of extra response edits ($\text{NED} \geq 0$)
**NUP** = maximum number of upscatter groups ($0 \leq \text{NUP} \leq \text{NGROUP}$)
**NTABL** = table length ($\text{NED}+4+\text{NUP} \leq \text{NTABL} \leq \text{NED}+4+\text{NUP}+\text{NGROUP}$)
**NGROUP** = number of energy groups
**IPTOT** = NED+3 = position of total cross-section

Table 1: Transport Table Terminology
Figure 1: Arrangement of neutron (n) and photon (g) cross sections in a coupled transport table with no upscatter.

Note that all the positions for group 1 are given first, followed by all the positions for group 2, and so on. The addition of sequence numbers on the right-hand edge of each card image goes back to the days when we worried about "dropping the deck."

III. COUPLED SETS

In fusion reactor analysis, it is very important to consider the energy transported by secondary photons. A convenient way to do this is to use a "coupled set." Because photon production from nuclear reactions is usually much stronger than neutron production from photon reactions, the normal down-scatter structure of the transport table can be preserved by considering photons as low-energy neutrons. This is done by defining a composite group structure with N neutron groups arranged as groups 1 through N, and G photon groups attached as groups N+1 through N+G. This arrangement is shown schematically in Figure 1.

Including accurate heat production cross sections for both neutrons and photons is important for coupled sets. When a neutron reacts with a nucleus, it produces local heating as charged particles and nuclear recoil, but much of the energy is carried away by secondary neutrons and photons. These secondary neutrons and photons travel to other parts of the assembly and deposit their energy there. Neutron heating values (or KERMA factors) are included in MATXS
libraries as HEAT, and photon heating is included as GHEAT.

The following TRANSX input deck illustrates the construction of a coupled set that includes nuclear heating as a special response-function edit in position 1 of the table.

```
TEST 3 -- COUPLED SET
0 3 0 12 1 1 0 3 0 0
42 2 46 0 0 1 1 1 1 2
AL-27
* */
1 1 AL27/
HEAT
1 HEAT/ NN AND NG PART
1 GHEAT/ GG PART
STOP
```

The number “12” in card two defines this to be a coupled set composed of particles 1 and 2. Similarly, “123” would be a coupled set consisting of three particles. Note that the number of groups has been increased to 42 (this is a 30 x 12 set) and the table length has been increased to 30+12+3+1, or 46, in order to account for the one special edit position. This edit is defined in cards 8 and 9 to be the sum of HEAT and GHEAT, but because HEAT is zero in the photon group range and GHEAT is zero in the neutron group range, the desired 42-group heating vector is obtained.

The output listing for this case is very similar to the one shown above, except that there are more groups. If one were to look at the structure of the scattering matrix, it would look much like the schematic in Figure 1. Position 5 and group 31 would be the scattering from gamma group 1 to gamma group 1; position 6 and group 31 would be the photon production in gamma group 1 from neutron group 30; and so on.

The CARD format output files from a case like this contain many zeros, as demonstrated by the example given above. One way to reduce the size of the file is to remove a range of n zeros by giving one zero and telling the code to repeat it n times. This is the principle behind FID0 format. An example follows:

```
AL-27 P0 48X 42 TABLE
4653210+0 -125012-5 0+0 1370375-6 1351484-741R 0+0 1
4782240+0 -131070-5 0+0 1376953-6 1345396-7 1579231-7 2
40 +0 0 4172990+0 -137062-5 0+0 1381831-6 1905282-7 3
1645201-7 4424638-839R 0+0 3024020+0 -145318-5 0+0 4
1371997-6 2143595-7 1436256-7 6515704-8 4029538-838R 0+0 5
1525510+0 -136369-5 0+0 1347487-6 2446181-7 1603739-7 6
```
| 7063102-8 | 5850607-8 | 7195755-837R | 0+0 | 5759920-1 | -122417-5 | 7 | 0+0 | 1434576-6 | 3622378-7 | 2225035-7 | 8017640-8 | 7599577-8 | 8 | 9 | 8982138-8 | 8102227-836R | 0+0 | 4084920-1 | -883599-6 | 0+0 | 9 | 1744508-6 | 8566135-7 | 4623700-7 | 1966109-7 | 1720993-7 | 1862898-7 | 10 | 10 | 1666632-7 | 1343127-735R | 0+0 | 3420560-1 | -638745-6 | 0+0 | 11 | 2028880-6 | 1046920-6 | 3246704-7 | 1474078-7 | 9130571-8 | 8814697-8 | 12 | 12 | 8261931-8 | 7893741-8 | 8470648-834R | 0+0 | 2874570-1 | -364917-6 | 13 | 13 | 0+0 | 2313132-6 | 1499382-6 | 4769126-7 | 1361422-7 | 7847956-8 | 14 | 14 | 8011064-8 | 8681243-8 | 8326775-8 | 8076122-8 | 8362886-833R | 0+0 | 15 | 15 | 2669560-1 | -307741-6 | 0+0 | 2559227-6 | 1725467-6 | 4832581-7 | 16 | 16 | 1849302-7 | 8692354-8 | 7190158-8 | 7714831-8 | 8330080-8 | 7761375-8 | 17 | 17 | 7435174-8 | 9456514-832R | 0+0 | 2172310-1 | -250960-6 | 0+0 | 18 | 18 |

... 194298-10 773477-10 180186-09 294745-09 341299-09 610631-09 148 3984609-9 T AL-27 P1 46X 42 TABLE 0 4R 0+0 7017524-845R 0+0 8125727-8 4661932-844R 0+0 1 9476780-8 2160392-8 7284464-943R 0+0 8426693-8 1164834-8 2 1679946-8 1781043-942R 0+0 7731138-8 1291789-8 7736112-9 3 3577544-9 7805438-941R 0+0 1032401-7 3047903-9 4103799-9 4 6116635-9 8614960-9 1439684-940R 0+0 3001111-7 5313039-9 5 5

Note the entries like "41R" that tell the code that reads the FIDO file to repeat the zero 41 times. Also note the terminator "T" that appears at the end of each table.

**IV. REACTOR PIN-CELL LATTICES**

Many reactor cores are made up of fuel pins arranged in a lattice and immersed in a coolant and moderator material. A simple example of such a reactor is the BAPL-1 critical assembly, which is part of the Cross Section Evaluation Working Group (CSEWG) standard benchmark set. This assembly uses slugs of enriched uranium oxide in aluminum tubes arranged in a triangular pattern in water. This kind of problem is too complex to be solved in one step with ordinary transport codes. The normal procedure is to reduce the space and energy detail by doing a simplified calculation for a single pin cell, and then to use these simplified cell cross sections to do a calculation for the complete reactor. An example of how to do such a calculation using TRANSX follows.

*MASS GET TRANSX:/TRANSX/SRC2/TRANSX0
*MASS GET ODN:/XS/SCODE/MACH5/ODN11DE9
*MASS GET MATXS:/LIB696/MATXS12
*FILE NAME=INPUT
BAPL-2 INFINITE LATTICE CELL - 69 GROUPS - ENDF/B-VI 0 5 0 1 2 1 0 1 0 0/
FUEL CLAD MOD/
FUEL 300.  .7433 3  1.15 1.15/
CLAD 300.  .28093 -3/
MOD 300.  1.3244 -3/
  1 1 016 4.6946E-2 FREE/
  1 1 U235 3.112E-4 FREE/
  1 1 U238 2.3127E-2 FREE/
  2 2 AL27 5.171E-2 FREE/
  3 3 H1 6.676E-2 H2O/
  3 3 016 3.338E-2 FREE/
CHI TRD/
STOP
*TRANSX
*SWITCH OUTPUT OUT1QQQ
*COPY GOIS MACRIS
*COPY GOIS SNIEDT
*FILE NAME=ODWINP
  1
BAPL-2 INFINITE LATTICE CELL - 69 GROUPS - ENDF/B-VI
DIMENS= 2 69 8 3 3 3 3 40 T
XMES=  0.4864 0.5753 0.8675 XINT= 18 4 18
ZONES= 1 2 3 T
LIB= MACRIS T
ASSIGN= MATHS T
SOLIN= 1 1 0 0 3 SOLOUT= 1 0 0 0 0 0 0 1 NORM= 1. T
RZMFLX= 1 T
*ODW
*SWITCH ODNOUT OUT2QQQ
*FILE NAME=INPUT
BAPL-2 INFINITE LATTICE CELL - 69 GROUPS - ENDF/B-VI
 0 5 0 1 2 1 0 1 0 3/
 69 2 115 40 40 4 5 11 4 2/
CELL REFL U235 U238/
FUEL 300.  .7433 3  1.15 1.15/
CLAD 300.  .28093 -3/
MOD 300.  1.3244 -3/
REFL 300. /
  1 1 016 4.6946E-2 FREE/
  1 1 U235 3.112E-4 FREE/
  1 1 U238 2.3127E-2 FREE/
  1 2 AL27 5.171E-2 FREE/
  1 3 H1 6.676E-2 H2O/
  1 3 016 3.338E-2 FREE/
  2 4 H1 6.676E-2 H2O/
  2 4 016 3.338E-2 FREE/
  3 1 U235 3.112E-4 RC/
  4 1 U238 2.3127E-2 RC/
CHI TRD FISS CAPT/
  3 WFTOT/
  4 NG/
STOP
*TRANSX
*SWITCH OUTPUT OUT3QQQ
*COPY GOIS MACRIS

78
This example will be discussed in detail in the following subsections. It uses a simple command language (note the commands with "**" in column 1) to retrieve the files needed, to run TRANSX to prepare cross sections for the regions of a pin cell, to run ONEDANT to compute the fine group flux in the pin cell, to run TRANSX again to compute the homogenized cross sections for the pin cell, to run ONEDANT again to compute the flux for the entire reactor, and, finally, to save the output listing for the entire job.

A. Group Ordering

The first two examples in this report generated cross section tables arranged by material and Legendre order. This BAPL example uses groupwise ordering, which is the natural ordering used inside transport codes. In this scheme, the cross sections for the group and the elements for scattering into the group from groups at higher energies are given together for all materials and Legendre orders. This is very efficient, because the transport equation is solved by sweeping down from group 1 to lower energy groups, and it only needs to keep data for one group in memory at each stage. The interface file used for this example is "GOXS" (for group-ordered cross sections), which is equivalent to the files "MACRXS" and "SNXEDT" used by ONEDANT and TWODANT. Note how GOXS is copied to MACRXS and SNXEDT after each TRANSX run for this example. An extract of the group-ordered listing from TRANSX is shown below.
** GROUP 1 **

<table>
<thead>
<tr>
<th>POSITION</th>
<th>FUEL PO</th>
<th>FUEL P1</th>
<th>CLAD PO</th>
<th>CLAD P1</th>
<th>MOD PO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 CHI</td>
<td>2.749E-02</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>2 TRD</td>
<td>1.280E-01</td>
<td>0.0000E+00</td>
<td>6.684E-02</td>
<td>0.0000E+00</td>
<td>5.824E-02</td>
</tr>
<tr>
<td>3 ABS</td>
<td>1.579E-02</td>
<td>0.0000E+00</td>
<td>4.921E-03</td>
<td>0.0000E+00</td>
<td>5.214E-03</td>
</tr>
<tr>
<td>4 NUSIGF</td>
<td>1.016E-01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>5 TOTAL</td>
<td>2.078E-01</td>
<td>0.0000E+00</td>
<td>9.856E-02</td>
<td>0.0000E+00</td>
<td>1.198E-01</td>
</tr>
<tr>
<td>46 INGRP</td>
<td>1.102E-01</td>
<td>8.003E-02</td>
<td>4.516E-02</td>
<td>3.038E-02</td>
<td>2.782E-02</td>
</tr>
</tbody>
</table>

** GROUP 2 **

<table>
<thead>
<tr>
<th>POSITION</th>
<th>FUEL PO</th>
<th>FUEL P1</th>
<th>CLAD PO</th>
<th>CLAD P1</th>
<th>MOD PO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 CHI</td>
<td>1.097E-01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>2 TRD</td>
<td>1.486E-01</td>
<td>0.0000E+00</td>
<td>7.189E-02</td>
<td>0.0000E+00</td>
<td>7.872E-02</td>
</tr>
<tr>
<td>3 ABS</td>
<td>1.658E-02</td>
<td>0.0000E+00</td>
<td>9.441E-04</td>
<td>0.0000E+00</td>
<td>2.380E-03</td>
</tr>
<tr>
<td>4 NUSIGF</td>
<td>3.956E-02</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>5 TOTAL</td>
<td>2.641E-01</td>
<td>0.0000E+00</td>
<td>1.167E-01</td>
<td>0.0000E+00</td>
<td>1.752E-01</td>
</tr>
<tr>
<td>46 INGRP</td>
<td>1.677E-01</td>
<td>1.168E-01</td>
<td>7.171E-02</td>
<td>4.237E-02</td>
<td>5.998E-02</td>
</tr>
<tr>
<td>47</td>
<td>2.735E-02</td>
<td>1.713E-03</td>
<td>2.089E-02</td>
<td>4.914E-04</td>
<td>3.762E-02</td>
</tr>
</tbody>
</table>

** GROUP 3 **

<table>
<thead>
<tr>
<th>POSITION</th>
<th>FUEL PO</th>
<th>FUEL P1</th>
<th>CLAD PO</th>
<th>CLAD P1</th>
<th>MOD PO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 CHI</td>
<td>2.135E-01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>2 TRD</td>
<td>1.490E-01</td>
<td>0.0000E+00</td>
<td>8.431E-02</td>
<td>0.0000E+00</td>
<td>8.769E-02</td>
</tr>
<tr>
<td>3 ABS</td>
<td>1.326E-02</td>
<td>0.0000E+00</td>
<td>8.201E-05</td>
<td>0.0000E+00</td>
<td>1.521E-05</td>
</tr>
<tr>
<td>4 NUSIGF</td>
<td>3.424E-02</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>5 TOTAL</td>
<td>2.418E-01</td>
<td>0.0000E+00</td>
<td>1.436E-01</td>
<td>0.0000E+00</td>
<td>2.053E-01</td>
</tr>
<tr>
<td>46 INGRP</td>
<td>1.582E-01</td>
<td>9.368E-02</td>
<td>1.066E-01</td>
<td>5.880E-02</td>
<td>6.308E-02</td>
</tr>
<tr>
<td>47</td>
<td>3.627E-02</td>
<td>2.363E-03</td>
<td>2.294E-02</td>
<td>1.639E-03</td>
<td>5.352E-02</td>
</tr>
<tr>
<td>48</td>
<td>1.021E-02</td>
<td>6.038E-04</td>
<td>1.116E-02</td>
<td>1.627E-04</td>
<td>1.756E-02</td>
</tr>
</tbody>
</table>

Note that this example uses macroscopic cross sections from TRANSX in both ONEDANT runs. The cards “LIB= MACRXS T” and “ASSIGN= MATLS T” result in by-passing the mixing capability of the transport code. This is the best way to use TRANSX with ONEDANT for any problem needing self-shielded cross sections. In effect, TRANSX becomes a new input module for ONEDANT.

B. Self-Shielding

This version of TRANSX handles resonance self-shielding by using the well-known Bondarenko Method, or Background Cross-Section Method. Average
cross sections that conserve the reaction rates can be defined using

\[ \sigma_g = \frac{\int_g \sigma(E) \phi(E) \, dE}{\int_g \phi(E) \, dE}, \]

where \( g \) stands for the energy range of one group, \( E \) is the energy, \( \sigma(E) \) is a microscopic cross section at \( E \), and \( \phi(E) \) is the neutron flux at \( E \). In a large asymptotic system where the resonances are fairly narrow with respect to the average energy loss of scattered neutrons, the flux is expected to vary inversely with the macroscopic total cross section. Therefore, the flux in a mixture of a resonant material and a moderator material can be written as

\[ \phi(E) = \frac{C(E)}{\sigma_0 + \sigma_t(E)}, \]

where \( C(E) \) represents the average smooth behavior of the flux (typically, \( 1/E \)), \( \sigma_t \) is the total cross section for the absorber, and \( \sigma_0 \) is the moderator cross section per absorber atom. The background cross section \( \sigma_0 \) clearly controls the size of the dip in the flux caused by an absorber resonance. If \( \sigma_0 \) is large, say \( 1 \times 10^{10} \) barns, the flux varies like \( C(E) \). This case is called “infinite dilution.” If \( \sigma_0 \) is small with respect to the height of peaks in \( \sigma_t \), strong dips in the flux would be expected. These dips would cancel out some of the reaction rate due to the corresponding peak in \( \sigma_t \), thus resulting in a self-shielding effect. The advantage of this model for the flux is that the multigroup cross sections can be prepared in advance for a number of \( \sigma_0 \) and temperature values, using a code like NJOY. Problem-dependent effective cross sections are then prepared by a code like TRANSX that determines the proper value for \( \sigma_0 \) and interpolates in the cross-section library.

For a lump of a resonance material embedded in a large moderating region, escapes from the lump also increase the effective background cross section. This additional escape cross section is given by

\[ \sigma_{esc} = \frac{1}{N\ell}, \]

where \( N \) is the number density of the absorber, and \( \ell \) is the mean chord length in the absorber lump

\[ \ell = \frac{4V}{S}, \]
and where $V$ and $S$ are the volume and surface area of the lump (e.g., for a cylinder, $\ell = 2r$). As a typical example, consider a 1-cm rod of uranium oxide surrounded by a large region of water:

$$
\sigma_0 = \frac{.046 \text{ at/cm} \times 3.76 \text{ b/at}}{.023 \text{ at/cm} \times 1 \text{ cm}} + \frac{1 \text{ cm}}{.023 \text{ at/cm}} \\
= 7.52 \text{ b/at} + 43.48 \text{ b/at} \\
= 51.0 \text{ b/at}
$$

where .023 and .046 are the atomic densities of the $^{238}\text{U}$ and oxygen, respectively, and 3.76 barns is the oxygen cross section.

For a lattice of absorbing rods, some neutrons that escape from one rod may travel to another rod before scattering from the moderator nucleus. In a sense, this is equivalent to never having escaped from the first rod at all. This kind of reduction in the escape cross section is called a Dancoff correction. TRANSX offers several possibilities; the option for a cylinder in an hexagonal lattice by the Sauer approximation is appropriate for the BAPL-1 case.

The construction of the background $\sigma_0$ is handled automatically by TRANSX 2.0 based on the region specifications and the mix specifications. Referring the input deck given above, lines 9–11 define the three regions needed for the Sauer approximation (IHET=3). The first is assumed to be the fuel, the second must be the can, and the third is the moderator (all three are taken to be at a temperature of 300 K). The region volumes given here (i.e., .7433, .28093, and 1.3244) are used to compute the escape cross section and the volume ratios needed for the Dancoff correction. Negative values of IHET are used to indicate the additional regions in a cell. The information in lines 12–17 is used to compute the mixture part of $\sigma_0$ and the moderator cross section needed for the Dancoff correction.

C. Thermal Cross Sections

At energies below a few eV, the binding of atoms in gases, liquids, or solids begins to affect the scattering of neutrons. TRANSX handles this by replacing the normal elastic scattering cross section and matrix with either free-gas or bound-atom versions from the MATXS library. The bound-atom cross sections available in our ENDF/B-VI libraries are summarized in Table 2. As seen in lines 12 through 17 of the sample input, the hydrogen is treated as H in H$_2$O.
Table 2: Moderator materials on the ENDF/B-VI thermal data files. The names in parentheses give the binding state for the principal scatterer. For example, C in graphite, or H in water. The MATXS names are based on this binding condition. Elastic scattering can be either coherent (coh) or incoherent (iel). In either case, the MATXS name is constructed by appending a dollar sign ($).

<table>
<thead>
<tr>
<th>Material</th>
<th>MATXS</th>
<th>Elastic</th>
<th>Secondary</th>
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<tr>
<td>BeO</td>
<td>BEO</td>
<td>coh</td>
<td>none</td>
</tr>
<tr>
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<td>GRAPH</td>
<td>coh</td>
<td>none</td>
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<tr>
<td>C(polyethylene)</td>
<td>POLY</td>
<td>iel</td>
<td>free C</td>
</tr>
<tr>
<td>C6H6</td>
<td>C6H6</td>
<td>none</td>
<td>none</td>
</tr>
<tr>
<td>D(D2O)</td>
<td>D2O</td>
<td>free O</td>
<td>none</td>
</tr>
<tr>
<td>H(H2O)</td>
<td>H2O</td>
<td>free O</td>
<td>none</td>
</tr>
<tr>
<td>Zr(ZrHn)</td>
<td>ZRH</td>
<td>iel</td>
<td>H(ZrHn)</td>
</tr>
<tr>
<td>H(ZrHn)</td>
<td>ZRH</td>
<td>iel</td>
<td>Zr(ZrHn)</td>
</tr>
</tbody>
</table>

and all other materials are treated using free-gas scattering (FREE). The two “40” entries on card 7 of the input deck indicate that there can be up to 40 upscatter groups (see NUP in Table 1) and that the 40 low-energy groups will use a thermal treatment. This puts the thermal cut-off at 2.6 eV.

D. Spatial Collapse

The first invocation of ONEDANT computes \( k_\infty \) and the region-averaged flux moments in the form of a RZMFPLX standard interface file. The second TRANSX run recomputes the self-shielded cross sections for the regions and uses the input flux file to prepare cell-averaged cross sections for the fuel region. In addition, a set of cross section tables is prepared for a large water reflector. The transport tables for the CELL and REFL mixtures are passed on to ONEDANT through the MACRXS file. Note that special edit cross sections are defined for \(^{235}\text{U}\) and \(^{238}\text{U}\) capture and fission. They are called “region constituent cross sections” (RC) because they are set equal to the corresponding component cross sections from the fuel pin in region 1. These cross sections are ultimately passed on to the ONEDANT edit module by means of the SNXEDT file.
Finally, the CELL and REFL cross sections are used to compute $k_{\text{eff}}$ for a buckled cylindrical model of the entire critical assembly. The ONEDANT edit module is used to convert the special $^{235}\text{U}$ and $^{238}\text{U}$ cross sections into the two-group reaction rates needed to compute the various capture and fission ratios measured for the BAPL-1 assembly.

V. THE TRANSX FLUX CALCULATOR

The most significant shortcoming of TRANSX is the self-shielding model used for thermal systems. The approach described above is dependent on the Narrow Resonance (NR) approximation, which is violated for many important resonances below 200–300 eV. The approach also has trouble handling some important resonance-resonance interference effects. In addition, it breaks down for some complex reactor designs, such as those using concentric cylinders, or those using a mix of uranium and plutonium fuel pins. Although some of the problems associated with wide and intermediate-width resonances can be alleviated by using cross sections prepared using the NJOY flux calculator, it would be useful to have a more general method available in TRANSX.

One such method uses a direct calculation of the point-energy flux to compute new self-shielded cross sections inside TRANSX. It is assumed that the complex arrangement of pins and cells in a lattice can be reduced to a single equivalent multi-region cell. The flux in each region of such a cell can be computed using

$$\phi_i(E) = \sum_j \tilde{T}_{ij}^{\text{VV}} Q_j(E) V_j,$$

where $Q_j$ is the neutron source in region $j$ with volume $V_j$. Note that $\tilde{T}_{ij}^{\text{VV}}$ describes the transport from volume $j$ to volume $i$. This equivalent cell is normally a cylindrical cell with a white boundary condition. However, it could also contain different regions for uranium and plutonium pins with the coupling between the two different cells taking place through their common surfaces. Each actual region (for example, the fuel) can be divided into several subregions to provide a better representation of the $r$ dependence of the flux.

This kind of a direct pointwise calculation of the flux is practical for energies below about 200 to 300 eV. The fluxes above the breakpoint $E_2$ are assumed to be spatially flat and to have the asymptotic $1/E$ shape. The fluxes below the breakpoint are computed by sweeping down through $E$ until some lower
Figure 2: Flux vs region and energy for the BAPL-1 fuel pin produced using the experimental TRANSX flux calculator. The first three regions are in the fuel, the fourth is the clad, and the last three regions are in the moderator.

limit $E_1$ is reached (for example, 2 eV). The results are highly accurate and automatically account for all the problems of wide and intermediate resonance width, resonance-resonance interference, multiple absorbing regions, and complex interactions between adjacent cells. However, this kind of calculation is expensive if many regions and many energy points are needed. It is important to keep the energy grid as sparse as possible and to keep the breakpoint energy as low as possible. An example of the space and energy dependence of a flux computed in this way is shown in Figure 2.

Once the detailed flux is available, it can be used with the pointwise cross sections to compute new self-shielded effective cross sections and elastic scattering matrix elements. The experimental flux calculator module for TRANSX can handle up to 5 scattering groups and 5 Legendre orders. Light-material scattering matrices are not self-shielded.

The pointwise cross sections needed for the flux calculation are obtained from a CCCC-type interface file\textsuperscript{17} called RESXS produced by the RESXSR module.
VI. PROBABILITY-TABLE SELF-SHIELDING

In the higher part of the resolved resonance range (above $E_2$) and in the unresolved range, it is impractical or impossible to do a detailed flux calculation. However, if the widths of the resonances are narrow with respect to the average energy loss in neutron scattering, the source terms for the resonance materials can be replaced by their asymptotic values:

$$Q_j(E) = \frac{\Sigma_{pj}}{E} ,$$  \hspace{1cm} (6)

where $\Sigma_{pj}$ is the macroscopic potential scattering cross section for region $j$. The fluxes become

$$\phi_i(E) = \sum_j T_{ij}^{VV} (E) \frac{\Sigma_{pj}}{E} V_j ,$$  \hspace{1cm} (7)

which is only a function of $E$ and is not correlated with flux values above $E$.

In this situation, it is possible to convert the integral over $E$ into an integral over cross section. Taking only one total cross section for simplicity,

$$\int_g f(\sigma_i(E)) dE = \int F_i(\sigma_i) f(\sigma_i) d\sigma_i ,$$  \hspace{1cm} (8)

where $F_i(\sigma_i)$ is the probability of finding a total cross section between $\sigma_i$ and $\sigma_i + d\sigma_i$ in the energy range $g$; $F_i(\sigma_i)$ is called the “total cross section probability table.” Other reaction cross sections are averaged using

$$\int_g \sigma_x(E) f(\sigma_i(E)) dE = \int F_x(\sigma_i) f(\sigma_i) d\sigma_i ,$$  \hspace{1cm} (9)

where $F_x(\sigma_i)$ is the average value of $\sigma_x$ when the total cross section is between $\sigma_i$ and $\sigma_i + d\sigma_i$; this is the “conditional mean” for $\sigma_x$. This formalism is easily extended to a mixture of resonant and non-resonant cross sections, even if a particular isotope appears in more than one region, by assuming that the cross sections for different isotopes are statistically uncorrelated. Then, for example,

$$\int_g \phi_i(E) dE = \int \cdots F_i(\sigma_1) F_i(\sigma_2) \cdots \phi(\sigma_1, \sigma_2, \cdots) d\sigma_1 d\sigma_2 \cdots ,$$  \hspace{1cm} (10)

and

$$\int_g \sigma_1(E) \phi_i(E) dE = \int \cdots F_i(\sigma_1) F_i(\sigma_2) \cdots \sigma_1 \phi(\sigma_1, \sigma_2, \cdots) d\sigma_1 d\sigma_2 \cdots ,$$  \hspace{1cm} (11)
where \( \sigma_1, \sigma_2, \text{etc.} \), are the microscopic cross sections for all the materials found in the cell. The quotient of these two equations is the self-shielded cross section. In practice, the integrals are converted to quadrature sums, and it is not necessary to integrate over any cross sections that are essentially constant in this energy range like hydrogen, deuterium, oxygen, or carbon.

This approach greatly reduces the number of transport matrix calculations needed to compute a group constant. For example, for a system with \(^{235}\text{U}\) and \(^{238}\text{U}\) as the only major resonance materials, and assuming the probability tables for \(^{235}\text{U}\) and \(^{238}\text{U}\) each have eight points, only 64 different \( T \) matrix calculations are required per group instead of the normal hundreds or thousands that would be required if working in the energy domain. The cost is the loss of correlation between resonances in different isotopes and the neglect of intermediate-resonance effects (neither of which is normally too important in this high-energy range). Note that the cross sections for one isotope that appears in more than one region are correlated. The advantage of this approach over the Bondarenko method is that no shaky equivalence-theory relations are used. It can handle complex geometries, such as cells with concentric cylindrical fuel regions, that are not amenable to equivalence theory. Also, the total cross-section iteration that is used to approximate the effects of resonance-resonance interference in the Bondarenko method is no longer needed (it is expensive in TRANSX).

This calculation can be greatly accelerated by a careful ordering of the loops over materials and probability bins. The bins for the material whose fluctuations cause the largest changes in the total macroscopic cross sections are summed in the outermost loop. Inner loops are ordered for increasingly smaller fluctuations. For any ordered set of cross sections \( \sigma_1, \sigma_2, \sigma_3, \cdots \), the value of \( \phi(\sigma_1, \sigma_2, \sigma_3, \cdots) \) is only recomputed if the macroscopic cross section \( \Sigma(\sigma_1, \sigma_2, \sigma_3, \cdots) \) changes significantly. Therefore, sums over the probability bins for minor materials might not even require a recalculation of the flux (this is basically treating them at infinite dilution). When \( \sigma_1 \) is at its highest value, even fluctuations for major isotopes may not trigger a flux recalculation. In any case, the number of expensive collision-probability calculations is greatly reduced.

The probability tables for TRANSX are read from a CCCC-type interface file called PTAB produced by the new PTABR module of NJOY. This module uses ordinary NJOY PENDF (pointwise ENDF) cross sections in the resolved-resonance range, and it uses probability tables from the PURR module of NJOY in the unresolved energy range.
VII. CONCLUSIONS

TRANSX 2.0 is a very useful code for preparing effective cross sections for a wide range of applications in nuclear technology. Its usefulness is enhanced by clean, modern coding and easy portability to many computer systems. Revision control for use in QA (Quality Assurance) environments is handled by using our UPD code,\(^{18}\) which provides a uniform way for making code updates on all computer systems. Several different MATXS libraries are available for TRANSX 2.0, and a greatly enhanced library-maintenance code BBC makes it easier to modify libraries or to prepare subset libraries that allow TRANSX to run much faster. Future versions of TRANSX will become even more useful by providing increased accuracy for thermal reactor analysis and calculations for complex geometries.

VIII. REFERENCES


AN ITERATIVE METHOD TO SOLVE THE SLOWING DOWN EQUATION IN HOMOGENEOUS MEDIA

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An iterative scheme is developed to solve the neutron slowing down equation in an infinite homogeneous media. Results obtained are compared with SECOL and NJOY ones.

I. Introduction

In order to study the resonance absorption in details, an iterative method has been developed to solve the neutron slowing down equation [1]. We will restrict here to the case of fine structure equation resolution (LIVOLANT- JEANPIERRE formalism) [2] in infinite homogeneous media. The values of effective integral calculated from fine flux obtained by this iterative method, by the SECOL code [3] and by the flux calculator of GROUPR NJOY module [4] have been compared.

II. Resolution of the fine structure equation by an iterative method

We consider an infinite homogeneous mixture of two materials. The material 1 is light and scattering material (moderator) and the material 0 has resonances. The slowing down equation is written as:

\[ \Sigma(u) \phi(u) = \int_{u-\epsilon_1}^{u} \frac{\Sigma_{s1}(u') \phi(u') \exp \left[-(u-u')\right]}{1-\alpha_1} \, du' + \int_{u-\epsilon_0}^{u} \frac{\Sigma_{s0}(u') \phi(u') \exp \left[-(u-u')\right]}{1-\alpha_0} \]

(1)

where:

\[ \Sigma = \Sigma_0 + \Sigma_1, \quad \Sigma_0 \, \text{and} \, \Sigma_1 = \text{total macroscopic cross-sections respectively of material 0 and material 1} \]

\[ \Sigma_{s0} \, \text{and} \, \Sigma_{s1} = \text{scattering macroscopic cross sections corresponding respectively to materials 0 and 1} \]

\[ \alpha_i = \frac{(A_i - 1)^2}{(A_i + 1)^2} \]

\[ \epsilon_i = \ln \left(1/\alpha_i\right) = \text{lethargy maximum gain} \]
The LIVOLANT-JEANPIERRE formalism assumes the flux factorisation:

\[ \Phi = \varphi \psi \]  \hspace{1cm} (2)

where:

- \( \psi \): is the "macroscopic flux",
- \( \varphi \): is the "fine structure"

One shows that the fine structure \( \varphi \) satisfies to the following equation:

\[ [\sigma_e + \sigma_0(u)] \varphi(u) = \sigma_e + \int_{u-\epsilon_0}^{u} \frac{\sigma_{so}(u') \exp[-(u-u')] \varphi(u')}{1-\alpha_0} \, du' \]  \hspace{1cm} (3)

where \( \sigma_e = \Sigma_1/N_0 \) is the equivalent cross-section (dilution).

Let be:

\[ \lambda(u) = \int_{u-\epsilon_0}^{u} \frac{\sigma_{so}(u') \exp[-(u-u')] \varphi(u')}{1-\alpha_0} \, du' \]  \hspace{1cm} (4)

Then:

\[ \varphi(u) = \frac{\sigma_e + \lambda(u)}{\sigma_e + \sigma_0(u)} \]  \hspace{1cm} (5)

The iterative scheme is defined by:

\[ \varphi^{(n+1)}(u) = \frac{\sigma_e + \lambda^{(n+1)}(u)}{\sigma_e + \sigma_0(u)} \]  \hspace{1cm} (6)

\[ \lambda^{(n+1)}(u) = \int_{u-\epsilon_0}^{u} \frac{\sigma_e + \lambda^{(n)}(u')}{\sigma_e + \sigma_0(u')} \frac{\sigma_{so}(u') \exp[-(u-u')]}{1-\alpha_0} \, du' \]  \hspace{1cm} (7)

One can demonstrate the convergence of this iterative scheme.
III. Results and comparisons

Figure 1 give an example of the fine structure energy variation obtained by the iterative method for the 6.67 ev U238 resonance. The variation of the $\lambda(u)$ is also shown.

Table 1 compare the values of effective integral:

$$I_{eff} = \int_{u_1}^{u_2} \sigma_a(u') \phi(u') \, du'$$

performed by the codes SECOL [3] and the GROUPR module of NJOY/Themis [4,5]. A good agreement is obtained in all studied cases with SECOL code. At low dilution values, there is an important discrepancy with NJOY/Themis. Others calculations will be made to well explain these differences.

The iterative method appears 4 times faster than SECOL. Time comparisons must be done with flux calculator of NJOY.

The iterative method has been generalized to the problems with source and several resonant nuclei and allows to study the mutual self-shielding.

We are studying the interest of implementation of this method in GROUPR NJOY/Themis module.

References


Figure 1: Variations of the fine structure, $\sigma_a$, $\sigma_s$ and $\lambda$ versus energy in the case of the 6.67 ev U238 resonance; $T = 20^\circ C$, $\sigma_e = 1000 b$.

Table 1: Comparisons of U238 $I_{\text{eff}}$ values obtained by three different methods – 2.77 ev - 4 KeV.

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>Method</th>
<th>$\sigma_e(b)$</th>
<th>$I_{\text{eff}}(b)$</th>
<th>$\Delta(%)$</th>
<th>$I_{\text{eff}}(b)$</th>
<th>$\Delta(%)$</th>
<th>$I_{\text{eff}}(b)$</th>
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$\Delta = \frac{\text{ITERATIVE} - \text{METHOD}_i}{\text{ITERATIVE}}$; $i = \text{SECOL, THEMIS}$
THE MONTE CARLO NEUTRON TRANSPORT CALCULATION USING THE PROBABILITY TABLE METHOD FOR CROSS-SECTIONS

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The probability table method has been developed for treating the neutron cross section in the resonances region. The advantage of this method is to represent properly the neutron cross section fluctuations within an energy group, allowing a correct calculation of the self-shielding. It has been used for multigroup and Monte Carlo calculation, also for the neutron slowing down calculation even though it is less exact in the resolved resonances energy range. In this paper, an application of the probability table method in the Monte Carlo neutron transport calculation has been developed to study the difference between the multigroup-probability table method and the traditional multigroup method; then the probability table method is introduced in the general Monte Carlo transport code TRIPOLI3. Finally, some examples calculated by the Monte Carlo method using the two models (multigroup-probability table model and multigroup model) are represented.

keywords: probability table, self-shielding, Monte Carlo method
I. Introduction

For a neutron transport calculation, the neutron cross section in the resonances region can be represented by several ways:

The pointwise method (Fig. 1a)---the cross section are defined by the interpolation between two points after the determination of the neutron energy; the advantage of this method is that during the neutron transport process, different values of the cross section are used in the energy interval, and the neutron has been transported more correctly, but it requires the enormous number of cross section and the calculation time will be very long in the practical calculation.

The multigroup method (Fig. 1b)---an averaged group cross section is defined in a given energy group, the neutron has always the same cross section within an energy group and the number of the cross section will be reduced; but it is very difficult to define the average cross section to represent correctly the self-shielding effect, even using a great number of energy group, because there are many resonances in the unresolved resonances region and the increase of the number of groups will just produce several groups having the same cross section.

The multigroup-probability table method (Fig. 1c)---not only the energy group, but also the cross section step in each group is defined in this method. The neutron can interact with more than one cross section in each group and the self-shielding effect will be more correctly represented than with the traditional multigroup model.

To use the multigroup-probability table method, it is necessary to create the probability table for each energy group and each isotope; several papers representing the probability table have been published by M.N.NICOLAEV\textsuperscript{1}, L.B.LEVITT, D.E. CULLEN\textsuperscript{2,3,4} and P.RIBON\textsuperscript{5}. The programs CAENDF\textsuperscript{6} and GROUPIE\textsuperscript{4} allow to calculate the probability table for each isotope. This cross section representation method has been used for the multigroup calculation, the Monte Carlo calculation and the neutron slowing down calculation\textsuperscript{7,8,9,10} even though it is more difficult to process properly in the resolved resonances region than in the unresolved resonances region. In this paper, a Monte Carlo neutron transport simulation using the probability table created by the program CAENDF\textsuperscript{6} is developed to study the difference between the probability table method and the traditional multigroup method; the Monte Carlo simulation method is the same as in the multigroup method because the multigroup transport equation can be extended to the multigroup-probability table equation (or multigroup-
multiband transport equation\(^3\)). Also, the multigroup-probability table method is introduced in the general Monte Carlo transport code TRIPOLI-3\(^1\).

II. The mathematic description of the probability table

In the program CALEND\(^6\), the conservation of the moments \(M_n\) of the total cross section is used to define the probability table. For a given energy group, the total cross section moment is defined by both the RIEMANN and the LEBESGUE integrals:

\[
M_n = \frac{1}{\Delta E} \int_{\Delta E} \sigma_t(E) \, dE
\]

or

\[
M_n = \int_{\Delta E} \sigma_t^p \, d\sigma_t
\]

where \(n\) is positive or negative, \(\sigma_t\) is the total cross section and \(p(\sigma_t) \, d\sigma_t\) is the probability of the total cross section between \(\sigma_t\) and \(\sigma_t + d\sigma_t\).

The integral of equation (2) can be transformed into a Gauss quadrature:

\[
M_n = \sum_{i=1}^{N} p_i \sigma_{t_i}
\]

where \(i=1,2,...,N\) is the cross section step number, \(p_i, \sigma_{t_i}\) are the probability and the total cross section for the cross section step \(i\).

There are \(2N\) unknown values \((p_i, \sigma_{t_i})\) in the system (3), it can be solved by defining \(2N\) values of the moments \(M_n\).

The partial cross sections \(\sigma_x\) are defined by:

\[
P_{x,m} = \frac{1}{\Delta E} \int_{\Delta E} \sigma_x \, \sigma_{t_i}^m(E) \, dE
\]

\[
= \int_{\Delta E} \sigma_x \, \sigma_{t_i}^m \, p(\sigma_t) \, d\sigma_t = \sum_{i=1}^{N} p_i \sigma_{x_i} \sigma_{t_i}
\]

The \(N\) values of these "partial moments" are necessary to resolve the system (4) to calculate the partial cross sections \(\sigma_{x_i}\) for each cross section step.

From the results of the two systems (3) and (4), the total and partial cross section are always maintained for each cross section step,

\[
\sum_{i=1}^{N} \sigma_{x_i} = \sigma_{t_i} \quad \text{and} \quad \sum_{i=1}^{N} p_i = 1
\]

A probability table is defined by the set \((p_i, \sigma_{t_i}, \sigma_{x_i})\), \(i=1,2,...,N\) for each energy group and each isotope, where \(N\) is the number of cross section steps. With these tables, the number of steps can be reduced (implying an accuracy decrease); the energy groups can be condensed and the probability table of a mixture can be determined from the probability table of each component of the composition.

III. Development of the multigroup-probability table method in the Monte Carlo neutron transport simulation.

The neutron transport problem is represented by the Boltzmann equation:

\[
\Omega \cdot \nabla \Phi(r,\Omega,E) + \Sigma_t(r,E)\Phi(r,\Omega,E) = R(r,\Omega,E)
\]

where \(\Phi(r,\Omega,E)\) is the flux in position \(r\), direction \(\Omega\) and energy \(E\), \(\Sigma_t(r,E)\) is the macroscopic total cross section in position \(r\) and energy \(E\), and

\[
R(r,\Omega,E) = \frac{1}{4\pi} \int_{0}^{2\pi} d\Omega' \int_{-\infty}^{\infty} dE' f(r,\Omega' \rightarrow \Omega,E' \rightarrow E) \Phi(r,\Omega',E')
\]

\(f(r,\Omega' \rightarrow \Omega,E' \rightarrow E)\) is the transfer distribution of the neutron scattered from direction \(\Omega'\), energy \(E'\) to direction \(\Omega\) and energy \(E\).
The multigroup transport equation is obtained by integrating over the energy in the group:
\[ \Omega \nabla \Phi_g(r,\Omega) + \Sigma_{T_g}(r)\Phi_g(r,\Omega) = R_g(r,\Omega) \] (7)
where \( \Phi_g(r,\Omega) \) is the flux in position \( r \), direction \( \Omega \) of the group \( g \), \( \Sigma_{T_g}(r) \) is the macroscopic total cross section in position \( r \) of the group \( g \), and
\[ R_g(r,\Omega) = \frac{1}{4\pi} \sum_{\Omega'} d\Omega' f(r,\Omega'\rightarrow\Omega,g'\rightarrow g)\Phi_{g'}(r,\Omega') \] (8)
\( f(r,\Omega'\rightarrow\Omega,g'\rightarrow g) \) is the transfer distribution of the neutron scattered from direction \( \Omega' \), energy group \( g' \) to direction \( \Omega \) and energy group \( g \).

The multigroup-probability table equation can be obtained by integrating over the energy and the cross section step in the group:
\[ \Omega \nabla \Phi_{g,i}(r,\Omega) + \Sigma_{T_{g,i}}(r)\Phi_{g,i}(r,\Omega) = R_{g,i}(r,\Omega) \] (9)
where \( \Phi_{g,i}(r,\Omega) \) is the flux in position \( r \), direction \( \Omega \) of the group \( g \) in the cross section step \( i \), \( \Sigma_{T_{g,i}}(r) \) is the macroscopic total cross section in position \( r \) of the group \( g \) in the cross section step \( i \), and
\[ R_{g,i}(r,\Omega) = \frac{1}{4\pi} \sum_{\Omega'} d\Omega' f(r,\Omega'\rightarrow\Omega,g' i'\rightarrow g i)\Phi_{g',i'}(r,\Omega') \] (10)
\( f(r,\Omega'\rightarrow\Omega,g' i'\rightarrow g i) \) is the transfer distribution of the neutron scattered from direction \( \Omega' \), energy group \( g' \), cross section step \( i' \) to direction \( \Omega \), energy group \( g \) and cross section step \( i \).

The narrow resonance approximation is used to define the transfer matrix; the probability that the neutron scatters from energy \( E' \) (group \( g' \)) to \( E \) (group \( g \)) is independent of the cross section at \( E' \) and \( E \), and is of cause independent of the cross section step number,
\[ p_{g,i\rightarrow g,i} = p_{g,i\rightarrow g,i} \] (11)
\( g \) and \( i \) are the group and the step number and the probability of the scattering from group \( g' \), cross section step \( i' \) to the group \( g \) and the cross section step \( i \):
\[ p_{g,i\rightarrow g,i} = p_{g,i\rightarrow g,i} \] (12)
where \( p_i \) is the probability of the cross section step \( i \) of the probability tables in the group \( g \).

Some important stages in the development of the simulation are:
1) The definition of the geometry, the material composition and the neutron source.
2) The definition of the total cross section which determines the neutron free path. For a composition of \( M \) isotopes, \( M \) random numbers are selected to choose the cross section step of each isotope in a given energy group,
\[ \xi_{1\rightarrow \text{cross section step } i_1 \text{ of isotope } 1} \]
\[ \xi_{2\rightarrow \text{cross section step } i_2 \text{ of isotope } 2} \]
\[ \ldots \]
\[ \xi_{M\rightarrow \text{cross section step } i_M \text{ of isotope } M} \]
the total cross section of the composition is:
\[ \Sigma_{c} = \sum_{j=1}^{M} \alpha_j \sigma_{ij} \] (13)
where \( \alpha_j \) is the number of atom per cm\(^3\) of isotope \( j \) (\( j=1,2,\ldots, M \)) and \( \sigma_{ij} \) is the total cross section of the isotope \( j \) in the cross section step \( i_j \).
3) The collision isotope is sampled by the probability
\[ p_j = \frac{\alpha_j \sigma_{ij}}{\Sigma_{c}} \]
4) The non-absorption probability is:
\[ p_{ni} = \frac{\sigma_{xij}}{\sigma_{xij}} \]

where \( \sigma_{xij} \) is the absorption cross section of the isotope \( j \) in the cross section step \( i \).

5) The reaction type is defined by the probability
\[ p_x = \frac{\sigma_{xij}}{\sigma_{xij}} \]

where \( x \) is the reaction type, \( \sigma_{xij} \) and \( \sigma_{xij} \) are the cross section of the reaction \( x \) and the scattering of the isotope \( j \) in the cross section step \( i \).

6) The anisotropic distribution is described in 32 intervals from -1 to 1, and is assumed constant inside each interval.

IV. Calculation examples and results

Example 1:
To study the influence of the number of cross section steps, the transmission probability of a slab (Fig.2) is calculated with one group approximation.

The thickness of the slab is \( n\lambda \) (\( \lambda \) is the mean free path of the neutron), the number of atoms per \( 10^{-24} \) cm\(^3 \) is 0.4955 and the macroscopic average total cross section is 1 barn. The neutron source is placed on the left side of the slab and normalized to unity.

![transmission probability](image)

Figure 2. Calculation example

The results are obtained by using the probability table with 1, 2, 3 and 4 steps (table 1) and compared with the results of the Sn method\(^{12} \) for the same example (Fig.3).

<table>
<thead>
<tr>
<th>( p_i )</th>
<th>( \sigma_{ti} )</th>
<th>( \sigma_{si} )</th>
<th>( \sigma_{ai} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 step</td>
<td>1.0000</td>
<td>2.0183E+0</td>
<td>2.0165E+0</td>
</tr>
<tr>
<td>2 steps</td>
<td>0.3836</td>
<td>1.4236E+0</td>
<td>1.4224E+0</td>
</tr>
<tr>
<td>3 steps</td>
<td>0.6164</td>
<td>2.3884E+0</td>
<td>2.3862E+0</td>
</tr>
<tr>
<td>4 steps</td>
<td>0.1751</td>
<td>1.2493E+0</td>
<td>1.2484E+0</td>
</tr>
<tr>
<td></td>
<td>0.4243</td>
<td>1.8526E+0</td>
<td>1.8509E+0</td>
</tr>
<tr>
<td></td>
<td>0.4006</td>
<td>2.5299E+0</td>
<td>2.5277E+0</td>
</tr>
<tr>
<td></td>
<td>0.0984</td>
<td>1.1838E+0</td>
<td>1.1823E+0</td>
</tr>
<tr>
<td></td>
<td>0.2508</td>
<td>1.5527E+0</td>
<td>1.5521E+0</td>
</tr>
<tr>
<td></td>
<td>0.3747</td>
<td>2.1209E+0</td>
<td>2.1183E+0</td>
</tr>
<tr>
<td></td>
<td>0.2761</td>
<td>2.5994E+0</td>
<td>2.5975E+0</td>
</tr>
</tbody>
</table>

\( p_i \): probability
\( \sigma_{ti} \): total cross section,
\( \sigma_{si} \): scattering cross section,
\( \sigma_{ai} \): capture cross section.

![Results of the probability table calculation](image)

Figure 3. Results of the probability table calculation
Example 2:

The influence of the number of energy groups in the multigroup-probability table model and in the traditional multigroup model is studied by the calculation of the transmission probability of a iron slab (number of atoms per $10^{-24} \text{ cm}^3 = 0.0846$) in the two models.

The neutron source is placed on the left side of an iron slab and normalized to unity, the source spectrum is uniform between 2.019 Mev and 1.653 Mev, the results between 2.019 Mev and 9.12 Kev are calculated by using 27, 54, 108, 216, 432, 1296, 2592 groups in the multigroup-probability table model (cross section library ENDF/B6) and 106, 2400 groups in the multigroup model (in this model, the result is obtained by the code TRIPOLI-311, cross section library UKNDL).

The table 2 gives the multigroup-probability table calculation results and the table 3 gives the multigroup calculation results, the comparison of the results is shown in figure 4.

Table 2. Multigroup-probability table calculation results.

<table>
<thead>
<tr>
<th>d (cm)</th>
<th>10</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>27 grs</td>
<td>0.961</td>
<td>0.34</td>
<td>0.925</td>
</tr>
<tr>
<td>54 grs</td>
<td>0.998</td>
<td>0.29</td>
<td>1.005</td>
</tr>
<tr>
<td>108 grs</td>
<td>0.998</td>
<td>0.29</td>
<td>1.005</td>
</tr>
<tr>
<td>216 grs</td>
<td>1.002</td>
<td>0.30</td>
<td>0.995</td>
</tr>
<tr>
<td>432 grs</td>
<td>1.000</td>
<td>0.27</td>
<td>1.000</td>
</tr>
<tr>
<td>1296 grs</td>
<td>1.004</td>
<td>0.28</td>
<td>1.005</td>
</tr>
</tbody>
</table>

* The values are the report of the transmission probability between the calculations of $n$ group and 2592 groups (the calculation of 2592 groups is considered as the reference).

Table 3. Multigroup calculation results

<table>
<thead>
<tr>
<th>d (cm)</th>
<th>10</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>106 grs</td>
<td>0.483*</td>
<td>0.111</td>
<td>0.021</td>
</tr>
<tr>
<td>2400 grs</td>
<td>0.522</td>
<td>0.149</td>
<td>0.042</td>
</tr>
<tr>
<td>106 grs</td>
<td>0.93</td>
<td>0.74</td>
<td>0.49</td>
</tr>
<tr>
<td>2400 grs</td>
<td>1.11</td>
<td>1.00</td>
<td>0.72</td>
</tr>
</tbody>
</table>

* The value is the transmission probability

Figure 4. Comparison of the different number of energy group in the two models (multigroup and multigroup-probability table)

p.t. --- probability table
tri --- TRIPOLI-3 (multigroup)

Discussion:

In the first example, the result of the one step is the same as the result of the Sn method but very different from the results of the two, three and four steps at great distance; in this case, the one step method and the Sn method used the same cross section, they have not considered the self-shielding effect and gave the smaller results. In the other hand, the more than one step models have treated the self-shielding effect and give the good results even with only two steps.

From the second example, the influence of the number of energy group is very important in the multigroup model at great
distance but not in the multigroup-probability table model because the self-shielding has been properly treated by the probability table. In practical, the probability table with a number of energy group reasonable will be very interesting for a calculation at great distance.

V Introduction of the probability table method in the general Monte Carlo transport code TRIPOLI-3

TRIPOLI-3 is a very general code\textsuperscript{11} to solve the transport problem in three dimensions by the Monte Carlo method. The multigroup model is used with 315 energy groups in the neutron shielding calculation.

In the multigroup-probability table model, we use always 315 energy groups, but the multigroup cross section is replaced by the multigroup-probability table cross section based on the neutron cross section libraries ENDF/B4 and JEF-2. The method to determine the mixture total cross section, the collision isotope, the reaction type, the anisotropic distribution and the non-absorption probability is the same as in the paragraph III.

One example is calculated by the TRIPOLI-3 program using the multigroup-probability table model: we consider a 100 cm iron slab (number of atom per $10^{-24}$ cm$^3$=0.0846), the neutron source is the same as in the second example of paragraph IV, the neutron currents are calculated in several distances. The neutron cross sections from the library ENDF/B4 are treated in 315 groups between 19.64 MeV and $10^{-5}$eV with an average 2 steps for each group. The multigroup model has been also used to calculate the same example by reducing the probability table into one cross section step. The results are demonstrated in table 4 and figure 5; the neutron spectra at 100 cm are also compared (Fig.6).

<table>
<thead>
<tr>
<th>d (cm)</th>
<th>1 step$^{(1)}$ J* $\sigma$(%)</th>
<th>m.steps$^{(2)}$ J* $\sigma$(%)</th>
<th>1 step m.steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.178 3.4</td>
<td>0.175 3.0</td>
<td>1.017</td>
</tr>
<tr>
<td>20</td>
<td>0.147 4.0</td>
<td>0.149 4.2</td>
<td>0.987</td>
</tr>
<tr>
<td>30</td>
<td>0.120 3.9</td>
<td>0.125 4.0</td>
<td>0.960</td>
</tr>
<tr>
<td>40</td>
<td>0.095 3.4</td>
<td>0.101 3.8</td>
<td>0.941</td>
</tr>
<tr>
<td>50</td>
<td>0.074 3.5</td>
<td>0.080 4.0</td>
<td>0.925</td>
</tr>
<tr>
<td>60</td>
<td>0.057 3.5</td>
<td>0.063 3.4</td>
<td>0.905</td>
</tr>
<tr>
<td>70</td>
<td>0.042 3.0</td>
<td>0.049 3.3</td>
<td>0.857</td>
</tr>
<tr>
<td>80</td>
<td>0.032 3.0</td>
<td>0.039 2.9</td>
<td>0.821</td>
</tr>
<tr>
<td>90</td>
<td>0.026 2.2</td>
<td>0.032 2.1</td>
<td>0.813</td>
</tr>
<tr>
<td>100</td>
<td>0.023 1.0</td>
<td>0.029 1.0</td>
<td>0.793</td>
</tr>
</tbody>
</table>

(1) 1 step=multigroup.
(2) m steps=multigroup-probability table.
* The values are the currents in each distance.

Figure 5. Results of the calculation by TRIPOLI-3 using the probability table method
VI. Conclusion

The probability table method for cross sections has been used in Monte Carlo neutron transport calculation. It allows to reduce the number of nuclear data and of the calculation time by comparing with the pointwise method, and represents more correctly the self-shielding effect than the multigroup method in which the self-shielding factor is very difficult to define.

From the results of the calculation, at small distance, there is no difference between the multigroup and the probability table models, but at great distance the difference become very important; the result is very sensitive to the number of energy groups in the multigroup model but not in the multigroup-probability table model.

References


11. J.C. NIMAL et coll, "Le programme de Monte-Carlo polycinétique à trois dimensions TRIPOLI-03", in publish.

Development of DRAGR for the Formatting of DRAGON Cross-section Libraries

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ABSTRACT

The DRAGR module was developed in NJOY-91 in order to put PENDF and GENDF nuclear data into a practical library format named DRAGLIB and adapted to the DRAGON lattice code. The DRAGLIB format is an attempt to define a simple and computationally efficient library structure that meets a set of requirements related to the peculiarities of thermal lattice calculations. More specifically, this study address the need for the DRAGR-DRAGON chain to provide identical results as the MATXSR-TRANSX chain for homogeneous domain neutronic calculations. Also, we established the need for the self-shielding data to preserve some normalization conditions. Finally, a tutorial will be given to explain how cross-section information should be extracted from a DRAGLIB file.

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I. INTRODUCTION

I.A. An Overview of the DRAGON Lattice Code

DRAGON\textsuperscript{1} is a new lattice code, based on integral transport theory, which provides the power to handle complex geometries which are typical of CANDU and PWR reactors whether the lattice is rectangular or hexagonal. DRAGON can use typical NJOY-compatible cross section libraries such as MATXS, APOLLIB-1 or DRAGLIB to produce properly interpolated and self-shielded macroscopic cross sections. DRAGON performs all the important functions required from a lattice code, including resonance self-shielding calculations, flux calculation with $K_{\text{eff}}$ or critical buckling search, isotopic depletion calculations and production of few group reactor properties. Self-shielding and flux calculations are performed in the exact 2D or 3D representation of the lattice cell. The code is built using advanced programming techniques which ensure modularity and facilitate maintenance. A simple hierarchical data base is provided to facilitate information exchange between modules, to collect important lattice parameters and to permit code restart.

The coding of DRAGON benefits from experience gained with other codes such as APOLLO-1\textsuperscript{2}, WIMS-AECL\textsuperscript{3} and TRANSX-CTR\textsuperscript{4}. DRAGON offers the possibility to use the APOLLIB-1 cross section libraries and to emulate most of the functionality of the APOLLO family of codes for treating PWR lattices. It also includes a fuel cluster model similar to the PIJ algorithm of the WIMS-AECL lattice code. This model is useful for the treatment of CANDU, AGR or RBMK lattices. Finally, DRAGON uses the same cross section representation as the code TRANSX-CTR for storing and using fission and scattering matrices. Both codes lead to the same neutronic results for the treatment of a homogeneous mixture of MATXS isotopes (some of them can be self-shielded).

I.B. An Overview of the DRAGR Module

As indicated in Fig. 1, many ways exist to input microscopic cross sections to DRAGON. The code accepts standard library formats such as MATXS (from NJOY-89 or NJOY-91), APOLLIB-1 and a specific format named DRAGLIB. Moreover, a utility exists in a development version of WILMA to transform a WIMSLIB library from WIMS-AECL to the DRAGLIB format. Utilities such as MATXS, THEMIS or WIMSR/WILMA can be used to produce MATXS, APOLLO-1 and WIMSLIB formats but these paths are not recommended for production work with DRAGON.

The DRAGR module was written as a clean and direct utility to format a DRAGLIB library, using PENDF and GENDF data. Care was taken to avoid unnecessary processing of nuclear data and to keep the richness of ENDF/B information. Other advantages are related to the use of the DRAGLIB format, thanks to the careful design of its direct access procedure.
II. The DRAGR Equations

II.A. Self-shielding Information

The goal of the self-shielding procedure is to evaluate \( \hat{\sigma}_y(g) \), the self-shielded microscopic cross section for a nuclear reaction \( y \). Here, \( \hat{\sigma}_y(g) \) is defined as

\[
\hat{\sigma}_y(g) = \frac{\int_{u_{g-1}}^{u_g} du \sigma_y(u) \varphi(u)}{\int_{u_{g-1}}^{u_g} du \varphi(u)} = \frac{I_y(g)}{\bar{\varphi}(g)}
\]

(1)

where

- \( u = \) lethargy = \( \ln(E_0/E) \) where \( E_0 \) is a reference energy
- index \( g = \) coarse energy group that may include many resonances and that will be used after completion of the self-shielding calculation
- \( u_{g-1}, u_g = \) lethargy limits of this group, with \( u_{g-1} < u_g \)
- \( \varphi(u) = \) fine structure function
- \( \sigma_y(u) = \) microscopic cross section for nuclear reaction \( y \)
- \( I_y(g) = \) effective resonance integral = \( \frac{1}{u_g - u_{g-1}} \int_{u_{g-1}}^{u_g} du \sigma_y(u) \varphi(u) \)
- \( \bar{\varphi}(g) = \) averaged fine structure function = \( \frac{1}{u_g - u_{g-1}} \int_{u_{g-1}}^{u_g} du \varphi(u) \)

DRAGON and codes of the APOLLO family assume that the fine structure function is the solution of an elastic slowing-down relation similar to the one found in the GROUPR flux calculator (with weight function IWT=3). In the lethargy domain, this equation can be written

\[
\sigma(u)\varphi(u) - \frac{1}{1 - \alpha_r} \int_{u - \epsilon_r}^{u} du' e^{u' - u} \sigma_s(u') \varphi(u') = \sigma_s(1 - \varphi(u))
\]

(4)

where

- \( \sigma(u) = \) total cross section of the resonant isotope
- \( \sigma_s(u) = \) scattering cross section of the resonant isotope
- \( \alpha_r = \left( \frac{A - 1}{A + 1} \right)^2 \) where \( A \) is the isotopic mass divided by the neutron mass
- \( \epsilon_r = \ln(1/\alpha_r) \)
- \( \sigma_e = \) dilution (expressed in barns) used as tabulation parameter.

This equation can be lethargy-averaged over group \( g \) to give the following balance relation:

\[
\bar{\varphi}(g, \sigma_e) = 1 - \frac{1}{\sigma_e} \left[ I(g, \sigma_e) - \sum_{h=1}^{g} \frac{u_h - u_{h-1}}{u_g - u_{g-1}} I_s(g \leftarrow h, \sigma_e) \right]
\]

(5)
where $I(g, \sigma_e) =$ total effective integral and $I_s(g \leftarrow h, \sigma_e) =$ scattering effective integral.

On the contrary to the MATXS format which stores directly the self-shielded cross sections $\bar{\sigma}_v(g, \sigma_e)$, other formats generally store effective integrals $I_v(g, \sigma_e)$. These integrals are tabulated as a function of dilution and absolute temperature. The goal of the self-shielding module in most lattice codes is to evaluate the actual dilution and to perform the required interpolations in the cross-section library. The result of this interpolation is the set of actual effective integrals that must be divided by the averaged fine structure function in order to obtain the required self-shielded cross sections. A few remarks can be made about this procedure:

1. The actual dilution in heterogeneous domains is computed in DRAGON using the generalized Stamm'ler method$^5$. This technique allows to treat arbitrary 2D and 3D geometries.

2. Effective integral interpolation performed in the lattice code should be polynomial in $\sqrt{\sigma_e}$ except for very large values of $\sigma_e$ where the interpolation should be linear in $1/\sigma_e$.

3. The averaged fine structure function $\bar{\varphi}(g, \sigma_e)$ is generally not written in the library. It must be computed in the lattice code using Eq. (5) for homogeneous calculations or using a similar expression for heterogeneous calculations, as indicated in Ref. 5.

The above procedure ensures that the same interpolated self-shielded cross sections will be produced for homogeneous domains, whether the MATXS-TRANSX or the DRAGON-DRAGON chain is used, provided that Eq. (5) is verified in NJOY. This condition is approximately satisfied by the GROUPR flux calculator but is actually not satisfied in the UNRESR module.

The following strategy was used in DRAGON to ensure that Eq. (5) is verified in every energy group. The averaged fine structure function $\bar{\varphi}(g, \sigma_e)$ computed in GROUPR is discarded and replaced by the solution of the following linear system of equations:

$$
\bar{\varphi}(g, \sigma_e) + \frac{1}{\sigma_e} \left[ \bar{\sigma}(g, \sigma_e) \bar{\varphi}(g, \sigma_e) - \sum_{h=1}^{g} \frac{u_h - u_{h-1}}{u_h - u_{g-1}} \bar{\sigma}_v(g \leftarrow h, \sigma_e) \bar{\varphi}(h, \sigma_e) \right] = 1
$$

(6)

The effective integrals are subsequently computed from

$$
I_v(g, \sigma_e) = \bar{\sigma}_v(g, \sigma_e) \, \bar{\varphi}(g, \sigma_e)
$$

(7)

where $\bar{\sigma}_v(g, \sigma_e)$ is the self-shielded cross section found on the GENDF file.

Averaged cross sections computed at infinite dilution (with $\varphi(u) = 1$) are then substracted from these values. The resulting values $\delta I_v(g, \sigma_e) = I_v(g, \sigma_e) - \bar{\sigma}_v(g, \infty)$ are written in the DRAGON library. This choice was made to save computer storage, since $\delta I_v$ is zero in each non resonant group.
II.B. Other Cross Section Information

The other multigroup microscopic cross sections produced by DRAGR follow the TRANSX-CTR methodology\(^4\). They are defined as follows:

1. The total cross section, \(\sigma(g)\), is edited from GENDF file.

2. The steady-state production cross section \(\nu\sigma_f(g)\) is calculated from GENDF file information, using

\[
\nu\sigma_f(g) = \sum_h \sigma_f(g \xleftarrow{} h) + \nu^D(g)\sigma_f(g)
\]  \hspace{1cm} (8)

where \(\sigma_f(g \xleftarrow{} h)\) is the group-to-group fission matrix, \(\nu^D(g)\) is the number of delayed neutrons per fission and \(\sigma_f(g)\) is the infinite dilution fission cross section.

3. The steady-state fission spectrum, \(\chi(g)\), is assumed to be dilution independent. It is calculated from GENDF file information, using

\[
\chi(g) = \frac{\sum h \sigma_f(g \xleftarrow{} h)\phi_0(h) + \chi^D(g)\sum h \nu^D(h)\sigma_f(h)\phi_0(h)}{\sum h \sigma_f(g \xleftarrow{} h)\phi_0(h) + \sum h \nu^D(h)\sigma_f(h)\phi_0(h)}
\]  \hspace{1cm} (9)

where the delayed spectrum is summed over the delayed energy groups;

\[
\chi^D(g) = \sum_{i=1}^{6} \chi^D_i(g)
\]  \hspace{1cm} (10)

and where \(\phi_0(h)\) is the library weight function for the first Legendre order.

4. The scattering matrix for the first Legendre order, \(\sigma_{\text{scat}0}(h \xleftarrow{} g)\), describes the energy transfer that follows an isotropic collision in the laboratory system. The collision can be an elastic or inelastic diffusion, a \((n,2n)\), or a \((n,3n)\) reaction. It is calculated from GENDF file information, using

\[
\sigma_{\text{scat}0}(h \xleftarrow{} g) = \sigma_{\text{diffusion}}(h \xleftarrow{} g) + \sigma_{2,2n}(h \xleftarrow{} g) + \sigma_{n,3n}(h \xleftarrow{} g)
\]  \hspace{1cm} (11)

This matrix is stored using the sparse storage scheme of the MATXS format, with the help of two \(h\)-indexed vectors:

\[
i_{\text{scat}}(h) = \text{most thermal group index that can produce a secondary neutron in group } h;
\]

\[
n_{\text{scat}}(h) = \text{number of primary groups that can produce a secondary neutron in group } h.
\]
1. CALL XSMOP(FILEM, IAC, IPRT) permits to open the library file, where
   \[
   \begin{align*}
   \text{FILENAME} & = \text{name of the library file} \\
   \text{IAC} & = 0: \text{for creating a new file;} \ 1: \text{for modifying an existing file;} \\
   & \quad \quad 2: \text{access in read-only mode (recommended for DRAGLIB access)} \\
   \text{IPRT} & = 0: \text{for no print on standard output;} \\
   & \quad \quad 1: \text{for information printing on standard output.}
   \end{align*}
   \]

2. CALL XSMSIX(NAMP, IACT) permits to move from one directory to an other one, where
   \[
   \begin{align*}
   \text{NAMP} & = \text{name of the target directory} \\
   \text{IACT} & = 1: \text{move to a son directory;} \\
   & \quad \quad 2: \text{move to the parent directory (NAMP can be set to a blank character).}
   \end{align*}
   \]

3. CALL XSMLEN(NAMP, ILONG, ITYPE) permits to obtain information regarding a block of information, where
   \[
   \begin{align*}
   \text{NAMP} & = \text{name of information block} \\
   \text{ILONG} & = \text{length of the information block (output)} \\
   \text{ITYPE} & = \text{type of the information block (output)} \\
   & \quad \quad 0: \text{sub-directory;} \ 1: \text{integer data;} \\
   & \quad \quad 2: \text{real data;} \ 3: \text{character*4 data.}
   \end{align*}
   \]

4. CALL XSMGET(NAMP, BLOCK) permits to recover a block of information, where
   \[
   \begin{align*}
   \text{NAMP} & = \text{name of information block} \\
   \text{BLOCK} & = \text{information recovered (output).}
   \end{align*}
   \]

5. CALL XSMCL permits to close the library file.

The DRAGLIB file contains the following data on its root directory:
1. a block named README containing character data describing the library;
2. a block named ENERGY containing the energy limits of the library;
3. a sub-directory named DEPL-CHAIN containing the burnup data for the depleting isotopes present in the library. This information include library names of the depleting isotopes in the chain, sums of radioactive decay constants, positions in chain of the parent nuclide and types of parent reaction, branching ratios for neutron induced or decay reactions, character names of the parent reactions, positions in chain of the fissiles isotopes, fission yields, and energies released per fission of each of the fissile isotopes;
4. one sub-directory for each isotope or material present in the library.

Each isotopic sub-directory contains the following information:

1. a block named README containing character data describing the isotope;
2. a block named AWR containing the value of the isotopic mass divided by the neutron mass;
3. a block named TEMPERATURE containing the values in Kelvin of the absolute temperature used in the cross section tabulation;
4. one sub-directory for each absolute temperature.

Each temperature sub-directory contains the following information:

1. one block for each of the following quantities: fission spectrum, total, production ($\nu\sigma$), scattering, fission, radiative capture, (n,2n) and (n,3n) cross sections evaluated at infinite dilution.
2. for resonant isotopes, a block named DILUTION containing the values in barn of the finite dilution used in the cross section tabulation.
3. for resonant isotopes, one sub-directory for each dilution. A dilution sub-directory contains one block for storing the $\delta I_p(g,\sigma_e)$ values of each self-shielded cross section.

We will now present a simple example to show the procedure that should be used to recover information from the DRAGLIB file. The following program permits to list the 69 energy group infinite-dilution radiative capture cross section of U-238 at temperature 900 K from a file named 'DRAGLIB':

```fortran
PROGRAM EXAMPLE
CHARACTER DIRECT*12
PARAMETER (MAXTMP=20,MAXNG=69)
DIMENSION TEMP(MAXTMP),XSNG(MAXNG)
CALL XSMOP('DRAGLIB',2,1)
CALL XSMSI6('U238',1)
CALL XSMLEN('TEMPERATURE',NTEMP,ITYPE)
IF(NTEMP.GT.MAXTMP) THEN
   PRINT *, 'MAXTMP SHOULD BE INCREASED TO ',NTEMP
   STOP
ENDIF
CALL XSMGET('TEMPERATURE',TEMP)
TEMP=0
DO 10 I=1,NTEMP
   IF(TEMP(I).EQ.900.0) ITEMP=I
10 CONTINUE
```
NSLINK: A code system to link NJOY to SCALE

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ABSTRACT

The INAS (JRI-NJOY-AMPX-SCALE) code system is used for criticality and reactor calculations. NSLINK is part of the INAS code system. It is a set of computer codes to convert the GENDF data from NJOY into SCALE-4 or SCALE-3 AMPX master format, retaining the Nordheim resolved resonance treatment option. Reich-Moore resonance parameters are converted to multi-level Breit-Wigner parameters. The AMPX master library is the basic library in both the SCALE-4 and SCALE-3 code systems. The AMPX master library can include data to use the Bondarenko, Nordheim or combined Bondarenko and Nordheim resonance treatment.
1. Introduction

The INAS system (IRI-NJOY-AMPX-SCALE) is a large system of FORTRAN 77 programs and nuclear data bases for reactor physics computations. Most of the codes originate from the Oak Ridge National Laboratory (ORNL) AMPX-SCALE package, and were adapted to run under the VAX/VMS operating system on a VAX cluster computer system. The basic data library for SCALE is the AMPX master library. This library is organized into one- and two-dimensional arrays by reaction type, scattering expansion order and energy groups. Also, Bondarenko self-shielding parameters and resonance parameters for the Nordheim resonance treatment can be included in the library. For both the SCALE-4 [1] and SCALE-3 [2] systems the format of the AMPX master library is the same. However, the definitions used for the resonance data are quite different.

In order to generate fine-group cross-sections with the NJOY [3] code and to put them in SCALE-4 or SCALE-3 AMPX master library format, a set of computer codes named NSLINK (NJOY-SCALE-LINK) has been developed. In the AMPX master library, data is included for further processing according to the Nordheim resonance treatment. Bondarenko self-shielding parameters can be generated as well. Resonance calculations can be done with the Bondarenko, Nordheim or combined Bondarenko and Nordheim resonance treatment using the BONAMI and/or NITAWL codes from the SCALE-4 or SCALE-3 code packages.

The AMPX master library can be generated with the XLACS and XLACS-2 codes [4] starting from ENDF/B or JEF files. However, the fine-group cross-sections generation code NJOY can treat different ENDF formats 3, 4, 5 and 6. The code includes more advanced options, is well-maintained and internationally accepted.

2. Overview of the NSLINK code package

NSLINK is part of the INAS computer code system. The following module and codes are included in the NSLINK code system:

- MILER: This is the basic code of the NSLINK system. The code is an extensively revised version of the original MILER [5] code. MILER converts output from NJOY (GEN‡F format) to AMPX master format. The code is used to generate master libraries used by the SCALE-4 or SCALE-3 system. No other module or codes are needed to generate a SCALE-4 master library.
• XLACSR: This module is only needed to generate master libraries used by the SCALE-3 system. The module (part of the NJOY code) is a stripped-down version of the XLACS-2 code. The necessary data for the Nordheim resonance treatment is generated by XLACSR.

• UNITABR: This code is only needed to generate master libraries used by the SCALE-3 system. The code is an adapted version of the UNITAB [4] code. It merges the output of XLACSR and MILER.

• BONAMI: In order to combine Bondarenko and Nordheim resonance treatment, some revised subroutines of the BONAMI code are included which replace the original ones. These subroutines are only needed for the version of BONAMI as used in the SCALE-3 system.

The flow diagram of NSLINK for SCALE-4 is shown in figure 1. The flow diagram of NSLINK for SCALE-3 is shown in figure 2.

The Netherlands Energy Research Foundation (ECN), in Petten, The Netherlands, contributed to the revision of MILER and tested the module and codes as well. They make use of NSLINK in the PASC (PETEN - AMPX - SCALE) computer code system.

3. The functionality of the module and codes

3.1 MILER

MILER is the basic code in the NSLINK system. The code converts a GENDF data library from NJOY to an AMPX master format as used in the SCALE-4 or SCALE-3 system. The modified GENDF format of NJOY91 can be read. Input instructions and definitions used to compute quantities in accordance with the definitions found in AMPX-2 are included as comment lines in the source code of MILER. The code is revised extensively and many additions have been made. Redundant cross-sections are checked for consistency. See for details the NSLINK User's Manual. [6] Bondarenko selfshielding factors can be generated and are then used over the whole energy range.

In case of generating an AMPX master for SCALE-4 and if Nordheim resonance data are intended to be used, the Bondarenko factors are set to 1 in the resolved energy range, except for the total cross-section MT=1, (iterative treatment in BONAMI). All Breit-Wigner resolved resonance data used in the Nordheim reso-
nance treatment are read from the original ENDF/B and JEF files. In an AMPX master for SCALE-4, only infinite dilution values of the group cross-sections are used.

The ENDF/B-VI and JEF 2.2 evaluations contain Reich-Moore (RM) resolved resonance parameters for some structural materials and the major actinides. The AMPX/SCALE code NITAWL which performs the Nordheim resolved resonance self-shielding treatment uses single-level Breit-Wigner (SLBW) parameters. The RM parameters are converted to multi-level Breit-Wigner (MLBW) parameters which are interpreted as SLBW parameters in the NITAWL code. [7]

In case of generating a SCALE-3 master the following codes and subroutines are also needed.

3.2 XLACSR

XLACSR is a stripped-down version of the XLACS-2 code. The module is included to generate the necessary data for the Nordheim resonance treatment in NITAWL as used in SCALE-3. XLACSR passes all $\ell = 0$ resonance parameters as well as the contributions from all other resonances to the group cross-sections, the contribution from the wings of the $\ell = 0$ resonances, the background cross-sections and possible interference for multi-level Breit-Wigner resonance parameters. The group cross-sections are stored in the appropriate 1-D cross-section arrays. (MT=1, 2, 18, 102, and the bodies of the resonances 1021, 1022 and 1023) The output file has AMPX-2 master format as used in the SCALE-3 system.

The original NJOY code is used to process all the nuclear data. The use of XLACSR does not affect the input to NJOY. In fact, if one does not want to use the Nordheim resonance treatment, the present NJOY version can still be used, with MILER to convert the output library of NJOY to the AMPX master library as used in the SCALE-4 or SCALE-3 system.

3.3 UNITABR

This code is an adapted version of the original UNITAB code which merges selected portions of AMPX master libraries into a new AMPX master library. [8] If resonance parameters for the Nordheim treatment are available then the code is used to generate an AMPX master library for the SCALE-3 system.

The output file of the XLACSR module (AMPX master format) is merged with the AMPX master file obtained from NJOY via MILER in such a way that group cross-sections of the bodies of the $\ell = 0$ resonances in the resolved energy range
(MT=1022 for fission and 1021 for capture), calculated by XLACSR, are subtracted from the infinite dilution values of the 1-D group cross-sections for fission (MT=18) and neutron capture (MT=102). The cross-sections of the bodies of the resonances (MT=1023 for elastic, 1022 and 1021) are added separately to the 1-D group cross-section arrays (MILER output). The redundant infinite dilution values of the total cross-sections (MT=1), the absorption cross-sections (MT=27) and the neutron disappearance cross-sections (MT=101) values are adjusted in the same way as for MT=18 etc.. The $\ell =0$ resonance parameters are included in the new AMPX master library.

If Bondarenko selfshielding data is available then the total cross-section values (MT=1) in the 1-D group cross-section arrays are copied before adjustment and added to the 1-D arrays as well. The reaction type identification is MT=2000. The Bondarenko factors and infinite dilution values of the total cross-sections (MT=1) in the Bondarenko data part of the AMPX master library are copied (MT=2000) for special (iterative) treatment in the BONAMI code. The infinite dilution values of the cross-sections (MT=1, 18 and 102) in the Bondarenko data part of the AMPX master library are adjusted in the same way as the cross-sections in the 1-D group cross-section arrays. Optionally the Bondarenko factors can be set to 1 in the resolved resonance energy region, discarding the selfshielding of the $\ell =1,2...$ resonances, the wings etc. The Bondarenko factors for MT=1 and 2000 are not changed, because of the iterative treatment in BONAMI.

The output file of UNITABR is in the AMPX-2 master format as used in the SCALE-3 system and includes resonance parameters for the Nordheim treatment or both Bondarenko and resonance parameters for the Nordheim treatment.

3.4 BONAMI

The revised subroutines of the BONAMI code which replace the original ones are only valid for the version of BONAMI as used in the SCALE-3 system.

BONAMI is the SCALE module which performs the Bondarenko resonance treatment for the nuclides containing Bondarenko selfshielding parameters. BONAMI allows the user to specify whether or not the code will iterate to determine the effective $\sigma_0$ value from previously shielded total cross-sections for all groups and zones in the problem. In the non-iterative case, BONAMI uses the potential scattering cross-sections to determine the effective $\sigma_0$ value. The iteration starts with the infinite dilution values of the total cross-sections of the nuclides. Using the NSLINC code system a nuclide may contain both Bondarenko selfshielding parameters and resonance parameters for the Nordheim treatment. If parameters for the Nordheim treatment are available, the total cross-sections MT=1 cannot be
used in the iterative process, because these cross-sections are adapted for the Nordheim resonance treatment to be performed later. Before correction, UNITABR copies the infinite dilution values of the total cross-sections and Bondarenko factors (MT=1 to MT=2000). If the total cross-sections MT=2000 are used instead of MT=1 this will be flagged in the printed output of BONAMI. If no resonance parameters for the Nordheim treatment are available, the original iterative method is not affected. The original input files for BONAMI can be used.

4. Benchmarking

Validation of code package and nuclear data that are used for criticality calculations are a continuous care of the reactor physics group. A number of standard criticality PWR and BWR reactor benchmarks are carried out to validate our 172 groups IRIJEF-1.3 (SCALE-3 format), IRIJEF-1.4 (SCALE-4 format) libraries and INAS code system including NSLINK. The JEF 1.1 evaluated data library and NJOY code version 89.62 have been used. The reactor benchmarks are partly done in cooperation with other Dutch institutes (ECN at Petten, GKN at Dodewaard and KEMA at Arnhem).

5. Status

- NSLINK version 3.0: includes conversion to SCALE-3 format libraries. Distributed to NEA DATA BANK and RSIC in May 1991.

- NSLINK version 4.0: reads GENDF format NJOY89; converts to SCALE-4 format libraries; all options as in version 3.0 retained. Not distributed.

- NSLINK version 4.1: reads new GENDF format NJOY91; converts RM parameters to MLBW resonance parameters; checks consistency of redundant cross-sections: all options as in version 4.0 retained. Will be distributed soon.

6. Conclusions

- The NSLINK modular code system, included in the INAS code system, is a powerful system to generate cross-section libraries used in the SCALE-4 and SCALE-3 code systems.
The use of SCALE-4 results in a quite simple NSLINK code system. The use of Bondarenko factors in the resolved resonance energy region is no longer needed as an option, when Nordheim resonance treatment is used. In this case the Bondarenko factors are set to 1.

ENDF format 6, including Reich-Moore resonance parameters can be used. Conversion to multi-level Breit-Wigner can be done.

NJOY89 or NJOY91 output (GENDF format) can be used as well.

References


DRAWBS - a graphics output module basing on GKS

S. Lehmann, M. Löchte, J.K. Axmann

Abstract
Today's computers offer good graphic facilities, however basing on a large number of different software products. The new NJOY module DRAWBS uses the graphic standard software GKS for outputs of ENDF, PENDF and GENDF files.

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1. Introduction

The merit of problem specific nuclear cross section production by a processing code like NJOY looses its benefits, if a new code and a not well tested cross section source like JEF-1 is used. Additional problems arise, if one is not very familiar with the use of NJOY or has installed a new part of the code. All of that can cause a considerable large number of errors, so that certainly almost every institution using NJOY knows about the problem of working with large ENDF, PENDF, and GENDF files without any reliability about correct results. A first step to increase the reliability of the evaluated nuclear data could be a visual control. Mainframes and workstations however often offer the possibility for graphical output, but with different software-products for nearly every operating system and computer. A typical example for this problem is the NJOY-module DTFR, that uses plotting subroutines, which are machine dependent and not available on many computers.

At the computer center of the Technical University of Braunschweig it was decided to develop every new output module more generally, basing on the Graphical Kernel System GKS, for nearly every graphics application. That gave rise to the Institute of Spaceflight- and Reactortechnology to write a new output subroutine for the DTFR module and to develop a new NJOY output module on basis of GKS.

2. Graphical Kernel System GKS

The Graphical Kernel System is an ISO-normed\(^1\) and hardware independent graphic software interface between the user software and the output hardware. It is compatible to the new software development PHIGS\(^2\) and is supported by many applications, because it allows to involve graphic-output modules, which are easy to transfer between different installations. These advantages are realized by a layer-structure of the system. (Picture 1)

---

\(^{1}\)International Organization for Standardization

\(^{2}\)Programmer's Hierarchical Interactive Graphics System
Concerning the applications, the GKS nucleus defines a set of computer-language independent functions. A language dependent layer allows an implementation of this system kernel in different programming languages – for example FORTRAN or PASCAL. Additionally it is possible to build up application dependent layers above the language layer. The graphical input and output devices are called graphical workstations. They are connected to the GKS nucleus by "device drivers", which not only generate an output for a special workstation, but handle the device dependent interaction, too. Every layer is able to call functions of the adjoining lower layer by an interface. (Picture 2)

Picture 2: Interfaces /1/
Some devices are:
- plotters (output workstations)
- digitizers (input workstations)
- interactive graphic terminals (input/output workstations)
- workstation independent segment storage (WISS)
- GKS-Metafiles (input/output)

GKS as a general-purpose graphical output software should be usable for most of the existing graphic devices and therefore by many applications - for example not only for normal plotting of static pictures, but also for the representation of dynamic motions. In addition GKS has to run on many hardware platforms with different central processing units, different storage handling or different processor word length. Therefore, GKS is not a fixed system, but designed in 9 suitable subsystems called levels. These levels are separated into two independent axes; the output level axis and the input level axis. The output and the input level axis allow the choice of three possibilities. For the output level one can find

0: a minimal output configuration
1: a basic segmentation with full output
2: a workstation independent segment storage

And for the input level one has the choice
a: for no input
b: for REQUEST input
c: for full input

The lowest level 0a allows a minimal configuration, which only contains a subset of the GKS functions and sets less requirements on the hardware. So, level 0a implementations can be installed on small computers - for example with 8 bit CPU's and slow external storage devices. The highest levels 2a, 2b and 2c contain all GKS features and need larger computers with at least 16 bit CPU’s, fast storage handling etc..

3. DTFR with GKS features

The first attempt to install an output module on basis of GKS at the Institute of Spaceflight- and Reactortechnology was carried out in 1990. The only reason for the implementation of the DTFR module was the possibility to produce graphical outputs of the cross section vectors and matrices. To use these graphical facilities on different output devices and not - like the original DTFR - on a special microfilm plotter only, it was necessary to rewrite the output subroutines in GKS. So for the implementation on the IBM 3090 at the Technical University of Braunschweig some standard
changes /3/ and some modifications in the output-routines had to be made. The work on the DTFR version for IBM computers is finished and this module can be requested from the institute or maybe from the NEA data bank.

4. The NJOY module DRAWBS

During the work on DTFR it seemed to be sensible to have a module, that produces dataplots in ENDF-format and even without the additional calculations of DTFR. The DRAWBS module is such a new utility for a graphical output of ENDF, PENDF and GENDF files in ASCII\(^3\) code for ENDF/B-V formats /2/. It bases on the lowest GKS level 0a, to guarantee a good compatibility for many computers. The input description is easy to handle and contains four cards: ( Picture 3 )

Card 1 defines some input/output parameters: NRPIC is the picture-number and IGRAPH the number of the graphs in the picture. The highest number for IGRAPH is 10. The variable ITYP describes the type of the data: 0 is used for a vector, 1 for a matrix and -1 presents the used positions in a matrix. IPRINT is a standard print option and IFILM characterizes, if there is no graphic output, black and white or a color output desired. ENBEG and ENLAST are the energy-boundaries with the default values 1.0E-5 eV and 2.0E7 eV.

Card 2 contains the graphic parameters. ISTYLE describes the text-style and NSCALE defines the kind of coordinate system to be used. The default value 0 chooses the double logarithmic scale. IGRID defines the scale options. For a vector (ITYP=0) no scale, grating, scale outside, and scale inside are available and for a matrix (ITYP=1) hidden lines, show all lines, scale outside, and scale inside can be chosen. IPOINT can be selected for PENDF-data only and defines whether the points are connected to each other by lines or not.

Card 3 only contains the picture title LABLE, defined as a string variable with maximal 60 characters.

Card 4 must be repeated for every graph in the picture (IGRAPH) and contains the material specifications. The first variable HISAM is an id-string with up to 4 characters. The next variable NIN refers to the number of the input unit. A zero for NIN means, that the last matrix datas should be used. MATD contains the desired material number (for example 4925 for U-235 from JEF-1). MTD and MFD describe the class of reaction MF and the class of data MT. The desired \(\sigma_0\)-value is given in JZD, the legendre-order in ML and the temperature in DTEMP. Additionally it is possible to show only one part of a matrix. This can be done by using ESTART or INGRP. ESTART defines the energy-group and INGRP the energy of the desired vector.

\(^3\)American Standard Code for Information Interchange
<table>
<thead>
<tr>
<th>card</th>
<th>variable</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NRPIC</td>
<td>picture-number (0: terminates, def.=0)</td>
</tr>
<tr>
<td></td>
<td>IGRAPH</td>
<td>number of graphs in the picture (max. 10)</td>
</tr>
<tr>
<td></td>
<td>ITYP</td>
<td>data type (0/1/-1: vector/matrix/matrix storage, def.=0)</td>
</tr>
<tr>
<td></td>
<td>IPRINT</td>
<td>print option (0/1: no print/print, def.=0)</td>
</tr>
<tr>
<td></td>
<td>IFILM</td>
<td>graphic type (0/1/2: no pic/black and white/color, def.=0)</td>
</tr>
<tr>
<td></td>
<td>ENBEG</td>
<td>lower energy limit (def. 1.0E-5 eV)</td>
</tr>
<tr>
<td></td>
<td>ENLAST</td>
<td>upper energy limit (def. 2.0E7 eV)</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>graphic parameters (only, if IFILM .ne. 0)</td>
</tr>
<tr>
<td></td>
<td>ISTYLE</td>
<td>text style (only, if ITYP = 0; ISTYLE .lt. 0 is italic)</td>
</tr>
<tr>
<td></td>
<td>NSCALE</td>
<td>coordinate system (0/1/2/3: log-log/lin-lin/lin-log/log-lin, def.=0)</td>
</tr>
<tr>
<td></td>
<td>IGRID</td>
<td>scale option (0/1/2/3)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ITYP = 0: no scale/grating-scale outside/scale inside</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ITYP = 1: hidden lines/show all lines/scale outside/inside</td>
</tr>
<tr>
<td>3</td>
<td>IPOINT</td>
<td>for PENDF-data (0/1/2: separate points/lines/points a. lines)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>picture title</td>
</tr>
<tr>
<td>4</td>
<td>LABLE</td>
<td>title; max. 60 characters</td>
</tr>
<tr>
<td></td>
<td>HISNAM</td>
<td>id-string; max. 4 characters</td>
</tr>
<tr>
<td></td>
<td>NIN</td>
<td>input unit (NIN .eq. 0: read from matrix storage)</td>
</tr>
<tr>
<td></td>
<td>MATD</td>
<td>material number</td>
</tr>
<tr>
<td></td>
<td>MTD</td>
<td>MT-number</td>
</tr>
<tr>
<td></td>
<td>MFD</td>
<td>MP-number</td>
</tr>
<tr>
<td></td>
<td>JZD</td>
<td>sigma zero (JZD .lt. 0 means: picture of the weight-flux)</td>
</tr>
<tr>
<td></td>
<td>ML</td>
<td>data position</td>
</tr>
<tr>
<td></td>
<td>DTEMP</td>
<td>desired temperature</td>
</tr>
<tr>
<td></td>
<td>ESTART</td>
<td>desired group-energy</td>
</tr>
<tr>
<td></td>
<td>INGRP</td>
<td>desired group-number</td>
</tr>
</tbody>
</table>

Picture 3: DRAWBS input cards /2/

5. The implementation of DRAWBS on IBM computers

The implementation of DRAWBS in the NJOY system depends on the local installation, but normally it is easy to handle. Only few changes have to be made in the main program of NJOY, to activate and call the new module (see: Appendix B). Some difficulties can result from the CPU word length and the I/O-unit definition.

At the Technical University of Braunschweig NJOY runs on an IBM 3090-600J with the operating system VM/XA. Because this computer is a short word machine, in all modules – including DRAWBS – many variables have to be declared as REAL*8 to get the desired precision /3/. This is
not necessary on other machines like CDC or Cray and should be remarked in this case. This can be done automatically by the code conversion program CCC.

The GKS implementation in Braunschweig uses the I/O-units 7 to 9 and 25 to 29, which therefore should not be used by NJOY. Additionally the output unit 6 is defined in GKS too, but it is possible to change the main output unit in the NJOY source code from 6 to 3 to keep the GKS output separately (see: Appendix B). One other correction is necessary in the NJOY subprogram REED to use I/O-units greater than 30. A data vector with the length of 30 for the units has to be changed to higher numbers (see: Appendix A).

6. Examples

Picture 4 shows an input card and the resulting DRAWBS output of the U-235 fission matrix in a 69 group structure for a temperature of 300 K. A special feature is shown in picture 5, which gives an overview of the U-235 fission matrix. Fields are marked in black, if the cross section in the matrix is greater than 1.0E-9.

![Picture 4: U-235 fission matrix](image)

```plaintext
*DRAWBS*
 1 1 1 1 1 /
 1 0 0 /
* FISSION MATRIX U235 ( 69 GROUP STRUCTURE; 300 K ) */
*GENP* 37 4925 18 6 1 0 300. /
0 /
*STOP*
```

Picture 4: U-235 fission matrix
Picture 5: U-235 fission matrix storage

The last picture 6 compares the total cross sections of U-235 from the PENDF- and the GENDF-file.

Picture 6: Total cross sections of U-235
7. Conclusion

The new DRAWBS module is a program for graphical output of NJOY data. It was designed for easy handling and uses the graphical kernel system GKS for the output, to realize implementations on many different computers.

Right now the module supports the ENDF/B-V format only, but if NJOY 91 and the JEF-2 data are installed at the Technical University of Braunschweig, the work on DRAWBS will be continued and it will be updated as soon as possible.

Additionally the DTFR module with its output routines on basis of GKS is now available and can be requested.

References


Appendix A

SUBROUTINE REED(N,IREC,I,L,MODE)
C ******************************
C READ A BINARY RECORD IN CCCC FORMAT.
C THIS IMPLEMENTATION SUPPORTS NON-CONSECUTIVE READING.
C ******************************
C
C Implicit REAL*8 (A-H,O-Z)
C
C DIMENSION X(L)
C DIMENSION IRL(30)
C DIMENSION IRL(99)
C IF (L.EQ.0) RETURN
C IF (IREC.GT.1) GO TO 110
C CALL REPO2(-N)
C GO TO 120
C 110 NSKP=IREC-IRL(N)-1
C IF (NSKP.NE.0) CALL SKIPRZ(-N,NSKP)
C 120 READ(N) (X(I),I=1,L)
C 130 IRL(N)=IREC
C RETURN
C END

Changes in subroutine REED
Appendix B

PROGRAM NJOY

C
C

***************NJOY NUCLEAR CROSS SECTION PROCESSING SYSTEM***************

C

C

EQUIVALENCE (DMOD,IMOD)
DATA STOP /4HSTOP/

C

C

DATA PLOT /4HPLOT/
DATA DRAW /4HDRAW/  

C

C

BEGIN DEFINE MAIN I/O UNITS
NSYSI=5
NSHORT=0
NSYSO=6
NSYSO=3  

C

C

IF (DMOD.EQ.STOP) GO TO 1000

C

C

IF (DMOD.EQ.PLOT) GO TO 270
IF (DMOD.EQ.DRAW) GO TO 280  

C

C

***PLOTR

C

C

***PLOT CROSS SECTIONS

C

C

270 CONTINUE
CALL PLOTR
GO TO 100

C

C

***DRAWBS

C

C

***GRAPHIC-OUTPUT

C

C

280 CONTINUE
CALL DRAWBS
GO TO 100

C

C

***NJJOY COMPLETE

C

C

Changes in the main program
Session 3:

GROUP CROSS-SECTION LIBRARIES
BENCHMARKING - APPLICATIONS

Chair:
Giancarlo Panini and Margarete Mattes
NEW DATA LIBRARIES FOR FAST BREEDER CALCULATIONS

by

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Abstract

We describe new ENDF/B-Ⅵ and JEF-1.1 based cross section libraries in the FDTAPE, GARTAPE, and GGTAPEx formats, and some results from the analysis of a large (1250 MWe) sodium-cooled fast breeder reactor benchmark. Pointwise and groupwise neutron cross sections in the ENDF/B like formats PENDF and GENDF have been prepared using NJOY (Edition 89.62), including double-differential scattering ENDF/B-Ⅵ cross sections in energy and angle. These files were edited into FDTAPE, GGTAPEx, and GARTAPE input files for the cell code MICROX-2, using the coupling and reformatting module MICROR. It is shown that good agreement (generally within one standard deviation) is achieved between the new results and the average values over sixteen benchmark solutions obtained in the past. The eigenvalues predicted with ENDF/B-Ⅵ are up to 0.7 % larger than those calculated with JEF-1.1 cross sections.
1 INTRODUCTION

In 1990 a series of calculations of a large (1250 MWe) sodium-cooled fast breeder reactor benchmark model (LMFBR benchmark) were performed at the Paul Scherrer Institute (PSI) [1] using nuclear data from Revision 1 of the Joint European File JEF-1.1 [2], processed with an old version of NJOY (Edition 83) [3].

The results showed good agreement, generally within one standard deviation, with the average values over sixteen benchmark solutions obtained in the past [4].

However, the Doppler-reactivity coefficient differed by about four standard deviations.

We therefore decided to recalculate the LMFBR benchmark using cross sections generated with a newer version of NJOY (Edition 89.62), and systematically processed the newest nuclear data files released, ENDF/B-VI [5], in addition to JEF-1.1.

In Section 2 of this report the new JEF-1.1 and ENDF/B-VI data libraries, including their processing scheme, are presented.

Section 3 reports the main results, and Section 4 gives some conclusions and recommendations.

2 NUCLEAR DATA

In this section we describe new ENDF/B-VI and JEF-1.1 based cross section libraries in the FDTAPE, GARTAPE, and GGTAPE formats, for the two-region spectrum code MICROX-2, an integral transport theory cell code originally developed for the efficient and rigorous preparation of broad group neutron cross sections for fast breeder reactors, which explicitly solves the neutron slowing down and thermalization equations on a detailed energy grid [6]. In addition, we describe new microscopic group delayed neutron precursor data files DLAYXS [7] for the first-order perturbation theory code PERT-V [8].

2.1 NJOY Libraries

Pointwise neutron cross sections in the ENDF/B like format PENDF have been prepared for the nuclides required in the LMFBR benchmark using the modules RECONR, BROADR, UNRESR, and THERMR of NJOY (Edition 89.62), which includes all updates of Edition 89.0 up to June 1990, and a modification in RECONR to the p-wave capture in ENDF/B-VI structural materials suggested by Eaton and Rowlands [9].

The RECONR module reconstructs pointwise (energy-dependent) zero temperature cross sections using ENDF/B resonance parameters and interpolation schemes. Resonance cross sections are calculated with an extended version of the methods of RESEND [10].

BROADR Doppler-broadens and thins pointwise cross sections using the method of SIGMA modified for better behaviour at high temperatures and low energies [11].

UNRESR computes effective self-shielded energy-, but not yet group-averaged cross sections in the unresolved-resonance region using the methods of ETOX [12].

RECONR (in Edition 89.62) is able to use the alternative Reich Moore formalism for treating the resolved energy range.

The PENDF files were generated using the JEF-1.1 and ENDF/B-VI evaluations.

The JEF-1.1 PENDF files consist of data for $^{10}$B, $^{11}$B, $^{12}$C, $^{16}$O, $^{23}$Na, natural chromium, iron, and nickel, $^{55}$Mn, $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, at 1100 K, and for $^{16}$O, $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, and $^{242}$Pu at 2200 K respectively.
The ENDF/B-VI PENDF files were processed for the same isotopes and temperatures as for JEF-1.1 except for the structural materials. The individual isotopes of chromium, i.e. $^{50}$Cr, $^{52}$Cr, $^{53}$Cr, $^{54}$Cr, of iron, i.e. $^{54}$Fe, $^{56}$Fe, $^{57}$Fe, $^{58}$Fe, and of nickel, i.e. $^{58}$Ni, $^{60}$Ni, $^{61}$Ni, $^{62}$Ni, $^{64}$Ni were generated, since there is no ENDF/B-VI data available for the natural structural elements.

Data for natural molybdenum was processed from JEF-2.0 due to some difficulties encountered in NJOY (Edition 89.62) when processing JEF-1.1 or ENDF/B-VI.

A PENDF file containing data for the inverse neutron velocities was produced from a pseudo JEF-1.1 nuclide generated at PSI using RECONR.

ENDF/B-VI and JEF-1.1 multigroup neutron cross sections in the GENDF format were generated from each PENDF file (including the PENDF file for the inverse velocities) with the GROUPR module, using the 193 neutron group structure from General Atomics [6]. The boundaries of the first 92 fast energy groups of the 193 neutron group structure used in MICROX-2 are taken from the GAM-II energy structure, whereas in the thermal range below 2.38 eV the boundaries are located between the 101 energy points of the GATHER-II code. The 92 fast energy group structure has 63 energy groups above 3.35 keV, i.e. 49 groups with lethargy width 0.10, followed by 14 groups with lethargy width 0.25.

In addition, JEF-1.1 GENDF files in 33 neutron groups were produced for $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, and $^{241}$Pu, and combined into a single GENDF file for use in obtaining 33 group delayed neutron precursor data DLAYXS.

In a similar way a GENDF file was generated including ENDF/B-VI data for the required actinides $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, and $^{242}$Pu.

The 33 neutron group structure, a sub-set of the 193 neutron groups, consists of a top group between 10 and 14.92 MeV, of 30 groups with constant lethargy width 0.5 between 10 MeV and 3.06 eV, and of two additional bottom groups between 3.06 and 2.38 eV, and 2.38 eV and 0.5 meV respectively, the group boundary at 2.38 eV being required in the MICROX-2 calculations.

The built-in input spectrum for fast breeder calculations (i.e. IWT=7 in the GROUPR terminology) was used for generating the multigroup cross sections.

The new automatic vector and matrix reaction options in GROUPR (i.e. 3/6) were used except for some fissionable isotopes (such as $^{235}$U in ENDF/B-VI), where there are still some inconsistencies in the availability of the fission reactions on the Files 3, 4, and 5 (in ENDF/B terminology).

GROUPR generates self-shielded groupwise vector cross sections, group-to-group neutron scattering matrices and photon production matrices using pointwise ENDF and PENDF data. The cross sections are written onto groupwise cross section files GENDF in ENDF/B like format. Vectors for all reaction types, matrices for reactions producing neutrons, including fission together with mixed data pertaining to fission yields of prompt and delayed neutrons can be generated.

The GROUPR format data sets in 193 neutron groups consist of shielded vector cross sections and $P_0$ through $P_4$ scattering matrices for all reaction types available on the PENDF files, which include double-differential scattering ENDF/B-VI cross sections in energy and angle (File 6 in ENDF/B terminology), and prompt and delayed fission, when appropriate. In addition, they contain data for the average cosine of the scattering angle, for the average energy decrement, and for the average square energy decrement (MT=251, 252, 253 in ENDF/B terminology).
Shielding factors were calculated in GROUPR using the narrow-resonance Bondarenko flux model. These refer to the isotope dependent sigma-zero tabulation given in Table 1. The sigma-zero values from Table 1 were empirically defined based on existing experience with fast breeder reactor calculations [13].

The GROUPR format data sets in 33 groups for the required actinides consist of infinitely dilute (sigma zero is equal to $10^{10}$ barns) vector cross sections and $P_0$ through $P_1$ scattering matrices, including prompt and delayed fission. $^{242}$Pu from JEF-1.1 could not be processed because there is no $^{242}$Pu delayed neutron data available in JEF-1.1.

2.2 MICROX-2 Libraries

GENDF files in 193 neutron groups and PENDF data files can be edited into the FDTAPE, GGTAPE and GARTAPE input files for MICROX-2 using the coupling and reformatting module MICOR (Version 2) [14] developed and maintained at PSI.

Corrections to an older version of the MICOR code (Version 1) used in a previous study [15] were applied to allow the FDTAPE and GGTAPE libraries to include an unlimited number of data sets (there was a limit of 50), and to eliminate an error leading to an unexpected truncation of the inelastic outscatter vectors particularly affecting $^{238}$U ENDF/B-VI fast data. Variable dimensions and consistent common blocks were introduced and replaced most of the fixed dimensions, especially in the GGTAPE section of the code.

The FDTAPE data file contains fine group dilution- and temperature-dependent cross sections in the fast energy range.

The GGTAPE data file consists of two sections which include infinitely dilute $P_0$ and $P_1$ cross sections in the fast and thermal energy ranges respectively. Only the pointwise thermal data portion of the GGTAPE data file is used by MICROX-2.

The GARTAPE data library contains pointwise, Doppler-broadened capture, fission, fission production ($\nu$ times $\sigma_f$), and elastic scattering resonance cross sections. Fine points up to about 9 keV, the threshold energy for $^{235}$U inelastic scattering, may be defined according to the criterion of equidistant lethargy or velocity spacing to be used in MICROX-2 for an accurate self-shielding of the resolved resonance range as a solution of slowing down equations in two zones.

Starting from the GENDF data in 193 groups and from the PENDF data described in the previous section, ENDF/B-VI and JEF-1.1, FDTAPE, GGTAPE, and GARTAPE data libraries suited for fast breeder reactor calculations were generated. In addition, FDTAPE, GGTAPE, and GARTAPE libraries were generated which contain cross sections from both the ENDF/B-VI and JEF-1.1 evaluations.

The FDTAPE data sets include 92 neutron group self-shielded cross sections up to $P_3$. Individual fission spectra for the actinides $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, and $^{242}$Pu, calculated in MICOR according to the methodology described in [16], were included in the FDTAPE and GGTAPE libraries.

The GARTAPE data libraries were generated on the basis of equidistant velocity spacing which results in a larger density of points at higher energies compared to the equidistant lethargy spacing, and the tabulation includes 11982 energy points between 2 eV and 2 keV.

2.3 Delayed Neutron Libraries

The JEF-1.1 and ENDF/B-VI GENDF files in 33 neutron groups were edited and reformatted into microscopic group delayed neu-
tron precursor data DLAYXS for the first-order perturbation theory code PERT-V using the NJOY module CCCCR, and converted to binary form using a management code developed for internal use at PSI. The DLAYXS format provides precursor yields, emission spectra, and decay constants ordered by isotope. Isotopes are identified by absolute isotope labels.

3 RESULTS AND DISCUSSION

We have analyzed the LMFBR benchmark model using the nuclear data libraries described in sections 2.1-2.3. In particular, we have calculated eigenvalues $k_{\text{eff}}$ and $k_{\infty}$, Doppler-reactivity coefficients, and central reactivity worths for various materials.

The required cell calculations were performed with a PSI version (Edition 14) of the code MICROX-2 from General Atomics. The upper limit for the pointwise slowing-down calculation was set at 582.947 eV, corresponding to the upper energy boundary for fine group 71 in the 193 group structure, and coinciding with the first fine group boundary below the upper bound of the resolved resonance range for $^{239}$Pu in JEF-1.1 (at 598 eV).

Since cross sections were processed with NJOY (Edition 89.62) this limit must be smaller than the minimum energy of the break between resolved and unresolved range over all important isotopes, such that the unresolved range can be shielded using the Bondarenko formalism [6].

This condition is needed because the unresolved resonance cross sections presently available on the GARTAPE library, coming from a sigma-zero tabulation originally done in UNRESR and obtained by averaging the cross sections over the unresolved resonance parameters, are energy-averaged cross sections given at infinite dilution. Therefore it was not possible to include the main sodium resonance (at about 2.5 keV) in the pointwise calculation.

The inner core $k_{\infty}$ calculations were performed with the one-dimensional discrete ordinates transport code ONEDANT [17], the full reactor forward and adjoint calculations with the two-dimensional discrete ordinates transport theory code TWODANT from Los Alamos, and the perturbation theory calculations with a PSI version of the first-order perturbation theory code PERT-V from Battelle-Northwest obtained from Los Alamos. We systematically used the 33 neutron group structure described before, which includes six additional groups compared to that defined in the original report [4], i.e. the top group between 10 and 14.92 MeV, and five groups below 13.71 eV.

Tables 2-4 summarize main results obtained using JEF-1.1 and ENDF/B-VI data, their relative deviations from the mean benchmark values, the standard deviations calculated from the sixteen benchmark solutions presented in [4], and the variation of the ENDF/B-VI results relative to the JEF-1.1 values.

Tables 2-4 prove that these new results generally lie within one standard deviation of average benchmark values.

Specific differences between the ENDF/B-VI and JEF-1.1 results include:

- the eigenvalues $k_{\text{eff}}$ for the eight configurations predicted with ENDF/B-VI are up to 0.7% larger than those calculated with JEF-1.1;
- the eigenvalue $k_{\infty}$ for the inner core of Configuration 1 significantly increases by 1.38 % when using ENDF/B-VI cross sections (i.e. 1.134 versus 1.119);
- the isothermal core fuel Doppler-reactivity coefficient agrees well within slightly more than one half of a standard deviation with the mean benchmark value. This is in contrast to the previous study done at PSI [1];
the effective delayed neutron fraction for Configuration 1 is 2.65% larger (i.e. 0.00392 versus 0.00382) when using ENDF/B-VI data;

- there are no significant differences between JEF-1.1 and ENDF/B-VI in the calculation of the central reactivity worths except for sodium. The rather big sodium worth in Configuration 3, calculated with JEF-1.1 data (about 1.3 standard deviations larger than the mean benchmark value), significantly decreases (by about 0.5 standard deviations) when using ENDF/B-VI cross sections (i.e. $-1.08 \times 10^{-6}$ versus $-1.01 \times 10^{-6}$ $\delta k_{eff}/k_{eff}/(10^{24} \text{ atoms})$).

4 CONCLUSIONS AND RECOMMENDATIONS

Using NJOY (Edition 89.62) we have generated new ENDF/B-VI and JEF-1.1 based cross section libraries in FDTAPE, GAR-TAPE, and GGTAPE format for the two-region spectrum code MICROX-2, and microscopic group delayed neutron precursor data files DLAYXS for the first-order perturbation theory code PERT-V.

We have then calculated a large (1250 MWe) sodium-cooled fast breeder reactor benchmark model, and compared eigenvalues, isothermal core fuel Doppler-reactivities, effective delayed neutron fraction, and reactivity worths with the average values over sixteen solutions obtained in the past.

From this study the following conclusions can be reached, and some recommendations can be made.

- Good agreement generally within one standard deviation is achieved between the new ENDF/B-VI and JEF-1.1 results, and the average values over the sixteen solutions obtained in the past. In particular, the calculated isothermal core fuel Doppler-reactivity coefficient now agrees well within about one half of a standard deviation with the mean benchmark value.

- Therefore, the new libraries as well as the methodology used in NJOY (Edition 89.62) for generating them seem to be adequate for calculations of "clean" fast breeder reactors.

- However, the module UNRESR should be modified in such a way that the unresolved energy range, and the main sodium resonance at 2.5 keV in particular, can be treated correctly in a detailed pointwise slowing down calculation.

- It is recommended to perform a similar study using cross sections generated with Edition 91 of NJOY.

References


<table>
<thead>
<tr>
<th>Isotope</th>
<th>Sigma-Zero Values (barns)</th>
</tr>
</thead>
<tbody>
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<td>$^{10}$B</td>
<td>$10^{10}$</td>
</tr>
<tr>
<td>$^{11}$B</td>
<td>$10^{10}$</td>
</tr>
<tr>
<td>$^{12}$C</td>
<td>$10^{10}$</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$10^{10}$</td>
</tr>
<tr>
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<td>$10^{10}$ 100 20</td>
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<td>$^{242}$Pu</td>
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Table 1: Sigma-Zero Values by Isotope in the GENDF Data Files
<table>
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<th>Data From</th>
<th>Eigenvalue</th>
<th>Std. Dev. (%)</th>
<th>Dev. from Mean Val. (%)</th>
<th>ENDF/B-VI Incr. Compared to JEF-1.1 (%)</th>
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<tr>
<td>Inner Core</td>
<td>Inner Core</td>
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Table 2: Eigenvalues $k_{eff}$ for the Eight Configurations, Eigenvalue $k_{in}$ for the Inner Core (Configuration 1), Calculated Using JEF-1.1 and ENDF/B-VI Data, and Their Deviations from the Mean Benchmark Values
<table>
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<th>Std. Dev. (%)</th>
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<th>Std. Dev. (%)</th>
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<td>-2.59</td>
<td>-721.4733</td>
<td>4.43</td>
<td>-2.78</td>
</tr>
<tr>
<td>$^{10}$B</td>
<td>ENDF/B-VI</td>
<td>-795.2034</td>
<td>5.43</td>
<td>1.75</td>
<td>-741.2405</td>
<td>4.43</td>
<td>-0.04</td>
</tr>
</tbody>
</table>

Table 3: Central Reactivity Worths Expressed in $\delta k_{eff}/k_{eff}/(10^{31}$ Atoms) Calculated Using JEF-1.1 and ENDF/B-VI Data, and Their Deviations from the Mean Benchmark Values

<table>
<thead>
<tr>
<th>Conf.</th>
<th>Data From</th>
<th>Fuel Doppler (%)</th>
<th>Std. Dev. (%)</th>
<th>Dev. from Mean Val. (%)</th>
<th>$\beta_{eff}$</th>
<th>Std. Dev. (%)</th>
<th>Dev. from Mean Val. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>JEF-1.1</td>
<td>-0.00740</td>
<td>10.80</td>
<td>1.56</td>
<td>0.0038227</td>
<td>2.62</td>
<td>-1.16</td>
</tr>
<tr>
<td>1</td>
<td>ENDF/B-VI</td>
<td>-0.00751</td>
<td>10.80</td>
<td>3.06</td>
<td>0.0039240</td>
<td>2.62</td>
<td>1.49</td>
</tr>
<tr>
<td>3</td>
<td>JEF-1.1</td>
<td>-0.00396</td>
<td>14.30</td>
<td>-8.64</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>3</td>
<td>ENDF/B-VI</td>
<td>-0.00430</td>
<td>14.30</td>
<td>-0.06</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
</tbody>
</table>

Table 4: Isothermal Core Fuel Doppler Reactivities and Delayed Neutron Fraction $\beta_{eff}$ Calculated Using JEF-1.1 and ENDF/B-VI Data, and Their Deviations from the Mean Benchmark Values
IAEA ACTIVITIES IN NUCLEAR DATA PROCESSING FOR THERMAL, FAST
AND FUSION REACTOR APPLICATIONS USING THE NJOY SYSTEM.

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ABSTRACT

The International Atomic Energy Agency has recently initiated a number of activities in
the area of nuclear data processing towards satisfying urgent needs of applied calculations. This
paper briefly summarizes the ongoing IAEA activities in nuclear data processing for thermal,
fast and fusion research and power reactor applications using the NJOY code system. The
activities that are described are (1) Processing of selected basic data libraries for elements of
interest to Agency’s program on Fusion Evaluated Nuclear data Library (FENDL); (2) Co-
ordination and participation in the WIMS Library Update Project (WLU Project) which aims
towards updating and improving the multigroup nuclear data input to the thermal reactor lattice
cell code WIMS; (3) Training activities in the use and applications of the NJOY system at the
IAEA Headquarters, Vienna, mainly for the IAEA fellowship applicants from IAEA Member
States; and (4) Verification of the accuracy of data processing using NJOY and other processing
codes that are available, i.e., the continuation of the IAEA nuclear data processing code
verification project. These four activities, all of which heavily use the NJOY system, are briefly
discussed in this paper.
1. INTRODUCTION

After a development period of 10-15 years, improved basic evaluated nuclear data libraries such as ENDF/B-VI, JENDL-3.1, BROND and JEF-2 have become available [1]. There are many reactor physicists around the world who are interested in updating and improving the multigroup nuclear data input to neutronic codes and point-data input to Monte-Carlo codes. The International Atomic Energy Agency has recently initiated a number of activities in the area of nuclear data processing toward satisfying the urgent needs of such calculations. This paper briefly summarizes the on-going IAEA activities in nuclear data processing for thermal, fast and fusion research and power reactors applications using the NJOY system. The IAEA activities on nuclear data processing consist of four different tasks which cover applied calculations for thermal, fast and fusion research and power reactors using NJOY [2-7] which is well known as the most general purpose and versatile nuclear data processing code system. These are as follows:

a. Using the NJOY to process selected basic data libraries for elements of interest to Agency’s program to develop a Fusion Evaluated Nuclear data Library (FENDL). The intermediate results can also be post-processed by the interested users for fast reactor applications.

b. Co-ordination and participation in the WIMS Library Update Project (WLU Project) which aims toward updating and improving the multigroup nuclear data input to the thermal reactor lattice cell code WIMS.

c. Training activities in the use and applications of NJOY at the IAEA Headquarters, Vienna, mainly for IAEA fellowship applicants from the IAEA Member States.

d. Verification of the accuracy of data processing using NJOY code system and other processing code systems that are available, i.e., the continuation of the IAEA nuclear data processing code verification project.

These four activities, all of which heavily use the NJOY system, are briefly discussed in this paper.
2. AGENCY’S PROGRAM ON FUSION EVALUATED NUCLEAR DATA LIBRARY (FENDL).

2.1 Introduction

The IAEA Nuclear data Section, in co-operation with several national nuclear data centres and research groups, is creating an internationally available Fusion Evaluated Nuclear Data Library (FENDL), which will serve as a comprehensive source of processed and tested nuclear data tailored to the requirements of the Engineering and Development Activities (EDA) of the International Thermonuclear Experimental Reactor (ITER) Project and other fusion-related development projects. The FENDL activity [8-10] is supported by several IAEA Coordinated Research Programmes. Within the scope of the FENDL project [8-10], the International Atomic Energy Agency is committed to a program of nuclear data processing activities in order to create a modern and internationally available Fusion Evaluated Nuclear Data Library (FENDL). Several materials from ENDF/B-VI, JENDL-3.1 and BROND basic files have been processed using the 32 bit IBM-3091 mainframe computer available at the IAEA. The nuclear data processing code system NJOY developed at Los Alamos National laboratory, USA [2-7] with all modifications and improvements as available in the NJOY version 89.80+ is employed in this study. A coupled neutron-gamma library for use in transport codes and a point library for use in Monte-Carlo code, in particular the MCNP code, will be produced and made freely available internationally to users as results of this program of nuclear data processing activity. The Nuclear Data Section has the goal of producing FENDL/M-1, a multigroup library in MATXS format, with a tentative target completion date of July 1992.

2.1 Source of basic data for FENDL:

The coupled neutron-gamma data files for elements and isotopes of FENDL will be derived from ENDF/B-VI, JENDL-3.1 and BROND for the following materials following the recommendation of the FENDL meetings [8-10]:

**ENDF/B-VI:** $^1$H, $^2$H, $^6$Li, $^7$Li, $^9$Be, $^{10}$B, $^{11}$B, C, $^{16}$O, $^{19}$F, P, S, Cl, K, $^{55}$V, $^{50,52,54}$Cr, $^{55}$Mn, $^{54,56,58}$Fe, $^{59}$Co, $^{58,60,62}$Ni, $^{63}$Cu, $^{134,136}$Ba, $^{182,184,186}$W, $^{206,208}$Pb.

**JENDL 3.1:** $^{23}$Na, Mg, $^{27}$Al, Ca, Ti, $^{55}$Mn, Mo, $^{181}$Ta, $^{209}$Bi.

**BROND:** $^2$H, $^{14}$N, $^{15}$N, Si, $^{90,92,94}$Zr, $^{91}$Nb, Sn.

2.2 Specifications for multigroup processing:

The specifications of multigroup processing as used in the NJOY runs for the FENDL project to produce a coupled neutron-gamma library is given below:

Neutron Groups: 175 (Vitamin-J structure)
Gamma groups: 42 (Vitamin-J structure)

Neutron weight function:

\[
\text{Thermal} + \frac{1}{E} + \text{Fission} + \text{Fusion} \ (IWT=6 \text{ in NJOY})
\]

Gamma weight function:

\[
\frac{1}{E} \text{ with rolloffs} \ (IWT=3 \text{ in NJOY})
\]

Legendre order for neutrons: \( P_5 \) for transport correction to \( P_3 \)

Legendre order for gammas: \( P_4 \) for transport correction to \( P_7 \)

Temperatures: 300, 900 and 1500 Kelvin

Dilution factors: \( 10^9, 10^4, 10^3, 10^2, 10^1 \), and \( 10^{10} \) barns

Reconstruction, linearization and thinning tolerances: 0.1 %

Thermal Scattering law included for Be in Be metal, C in graphite and H in water.

In spite of the limited manpower available for processing activities at the IAEA, evaluated files for most of the materials of FENDL have been successfully processed, and including up to the generation of Group ENDF or "GENDF" files. A coupled neutron-gamma library in MATXS format for use in transport codes and a point library for use in Monte-Carlo code, in particular the MCNP code, will be produced and made freely available internationally to users as results of this program of nuclear data processing activity. However, the progress towards this goal is hampered at the time of writing this report by compatibility problems between the GROUPR and MATXS modules of NJOY and between MATXS and TRAMIX (TRANSX) post-processing programs. The NDS will be obtaining consulting assistance from the NJOY and TRANSX author R.E. MacFarlane on these problems so that the above stated target completion date still appears realistic.

3. IAEA CODE VERIFICATION PROJECT

The section briefly reviews the present status of the activities of the IAEA nuclear data processing code verification project [11-13]. We present some typical samples of our comparisons of line shapes produced for FENDL materials by both NJOY 89.31 and RECENT to see if both these codes produce essentially identical results.

The main conclusions are that, with an IBM mainframe, one needs to employ double precision in NJOY for the energy variable, and that there are other ambiguities, in addition, in the ENDF/B basic file and in the processing of unresolved resonance region etc. Thus there are
are many data processing issues and related physics still to be addressed. In spite of all this, we feel that this project is making considerable progress toward its main goal, namely, to make the nuclear data processing codes much more reliable. The IAEA code verification project [11-13] is a continuing activity at the Agency and the verification exercise will extend to other modules of processing. Any one interested to participate in the processing code verification project should please contact the first author of this report. Note that the IAEA code verification project [11-13] is being carried out primarily through correspondence and at no cost to the Agency.

3.1 Accuracy of reconstruction of line shapes

In the comparisons presented here, a reconstruction tolerance of 0.1% was employed as input in each of the processing modules RECONR and BROADR of the NJOY code system and similarly in the case of D.E. Cullen’s codes LINEAR/RECENT/FIXUP/SIGMA1 [14-17].

3.2 Materials for which line shapes were compared

The following materials of ENDF/B-VI are covered:

\[ \begin{align*}
{^1}\text{H}, \quad {^2}\text{H}, \quad {^3}\text{H}, \quad {^6}\text{Li}, \quad {^7}\text{Li}, \quad {^9}\text{Be}, \quad {^{10}}\text{B}, \quad {^{11}}\text{B}, \quad {^{14}}\text{N}, \quad {^{15}}\text{N}, \quad {^{16}}\text{O}, \quad {^{19}}\text{F}, \quad {^{27}}\text{Al}, \quad {\text{Si}}, \quad {\text{Ti}}, \quad {^{55}}\text{V}, \quad {^{50,52,54}}\text{Cr}, \quad {^{55}}\text{Mn}, \\
{^{54,56,58}}\text{Fe}, \quad {^{59}}\text{Co}, \quad {^{58,60,62,64}}\text{Ni}, \quad {^{63,65}}\text{Cu}, \quad {^{90,92,94,96}}\text{Zr}, \quad {^{93}}\text{Nb}, \quad {\text{Mo}}, \quad {\text{Sn}}, \quad {^{134-138}}\text{Ba}, \quad {^{182-184,186}}\text{W}, \quad {^{206-208}}\text{Pb}, \quad {^{209}}\text{Bi}, \\
{^{241}}\text{Pu}, \quad {^{232}}\text{Th} \text{ and } {^{238}}\text{U}
\end{align*} \]

The IAEA pre-processing codes LINEAR/RECENT/FIXUP/SIGMA1 and NJOY code system should, in principle, produce identical results (i.e. cross section line shapes), as both these processing code systems start from the same basic data file ENDF/B-VI and employ similar resonance reconstruction strategies.

3.3. Main results of intercomparison

All line shapes were intercompared using the COMPLOT program [17] in considerable detail using, in many cases, the “zooming” option. The results are presented in Figs. 1-163 of the unpublished report [13] and are not reproduced to save space. We have communicated the main discrepancies to R.E. MacFarlane at Los Alamos, D.E. Cullen at Lawrence Livermore Laboratory, and C. L. Dunford at Brookhaven National Laboratory, USA. We would like to acknowledge with thanks D. E. Cullen and R.E. MacFarlane for their important contributions to and active collaboration in this code verification project and for other useful feedback. Some of the interesting observations are as follows:

The cross section line shapes produced by NJOY89.31 and Red Cullen’s codes LINEAR/RECENT/FIXUP/SIGMA1 showed, in general, in most of the energy regions, for most of the reactions in the case of most of the isotopes, excellent or perfect agreement. For
example, we see, for instance, in Fig. 1 and Fig. 2 that the results for $^{241}$Pu are in good agreement, except at the boundaries of resolved and unresolved resonance region. It should be borne in mind that both NJOY [2-7] and the IAEA codes [14-17] were developed over a period of 10-15 years and it is extremely satisfying that, for the newly released ENDF/B-VI file, these code systems produce essentially identical results for most of the nuclear reaction cross sections. Selected results of comparisons are presented where, in some of these graphs, there are differences that cannot be ignored. We stress that since these comparisons were made, NJOY89.31 has been updated by R.E. MacFarlane and presently NJOY91.13 is available for distribution by Radiation Shielding and Information Center, Oak Ridge National laboratory, U.S.A. With this version of NJOY most of the differences have been eliminated. However, if the reader is using an older version of NJOY, he/she may still encounter these problems.

a. Resolved resonance region; potential scattering cross section

One of the most interesting discrepancies occurred in the case of $^{207}$Pb as shown in Fig. 3. The potential cross section calculated by NJOY and RECENT differed substantially from each other. Cullen pointed to the fact that the large differences in the elastic cross section is due to different treatments of the j-multiplicity for both $L=1$ and $L=2$, which is adequately treated by RECENT. A memorandum clarifying the related issues is available from the authors [18].

b. Doppler broadening effects

The Doppler broadened line shapes at 300 Kelvin fail to achieve perfect agreement in many energy regions for many isotopes[13] but to save space we describe below only one interesting experience. More comparisons will be performed in the near future and results reported. The reason that the Doppler broadening aspects cannot be adequately presented here is that such discussions would be a premature mixture of the effects of differences in 300 Kelvin line shapes due to differences is zero Kelvin line shapes themselves plus differences if any due to the Doppler broadening modules themselves. In some cases the zero Kelvin cross sections agreed but not the higher temperature line shapes. Only one such sample is discussed below as a typical example: The 300 Kelvin (n, gamma) cross section data of $^{30}$Si (Fig. 4) showed up some new structures for some of the narrow peaks in the higher energy (MeV) region at 300 K as compared to zero K line shapes. This non-physical Doppler broadening effect was successfully traced to a bug in BROADR module of NJOY by R.E. MacFarlane. The bug has been corrected by R.E.MacFarlane already, and we confirmed that it does not occur with our NJOY 89.80+ version.

c. Effects due to precision of IBM

1) NJOY was designed to operate on long word-length computers such as CDC and Cray. 2) RECENT was designed to operate on either long word length computers using single precision arithmetic or on short word length computers. (e.g., IBM) using double precision arithmetic.
For $^{60}$Ni the NJOY results using double precision arithmetic on an IBM-3081 agree with
the NJOY-Cray and RECENT results, bringing us to a clear conclusion that the user of NJOY
should not use NJOY in single precision on IBM mainframe computers but go always to use
double precision. The IBM-3081 employs 32-bit arithmetic, and as a result, in the
reconstruction of sharp resonances in the resolved resonance region, NJOY is limited on this
machine to a maximum of 6 digits in the single precision representation of the energy variable,
whereas RECENT uses up to 9 digits of accuracy. We investigated this further in collaboration
with Riyanto Raharjo of Indonesia as follows. Using an automatic compiler option available in
IBM compiler, we created a double precision version of NJOY driver module and of RECONR,
and tested it for $^{60}$Ni data of ENDF/B-VI. The differences seen in Figs. 5-7 between
NJOY(RECONR) and RECENT for $^{60}$Ni essentially disappear when 7 digits are employed in the
double precision version of NJOY. The results for even-even actinides such as $^{233}$Th and $^{238}$U
distinctly showed the effect of using 9 digits in RECENT as compared to 6 digits in RECONR
in many sharp resonances. The implications of 6 digits on Doppler changes can be significant
as found earlier [12]. Figure 8 compares the results of a Cray run with 7 digits accuracy with
RECENT for a p-wave resonance in $^{233}$Th. The discrepancy (Fig. 9) almost disappears with the
use of 7 digits. In summarizing this section, we state that, in many cases of isotopes, for zero
Kelvin line shapes, NJOY(IBM-3081) differs significantly from RECENT unless double
precision is used. On the other hand, there are cases such as $^{241}$Pu where the resonances are not
so sharp as to demand more than 6 digits of accuracy. In such cases the NJOY(IBM) and
RECENT agree. See Fig. 1 and Fig. 2.

d. Unresolved resonance region

There were differences in the average 'point' cross sections calculated by the two
processing modules RECONR and RECENT at zero K in the unresolved resonance region
(URR) for some isotopes, namely, $^{238}$U, Mo, W, and $^{184}$W [Figs. 10-13]. In the case of Mo,
as shown in Fig. 11, differences of -5.71% to +3.2% is seen for (n, gamma) cross sections in
URR. For W, a clear discrepancy is seen (Fig. 12) in the unresolved resonance region. When
the cross sections calculated by NJOY and RECENT agree in the URR (as in case of last three
isotopes mentioned above) at only specific nodes, it can be deduced that the reason for the
differences in the URR is due to different procedures or logic followed by NJOY and
RECENT. Figure 10 gives the comparison for the $^{238}$U (n, gamma) cross section at zero degree
Kelvin. The 7% difference in the unresolved resonance region for capture was due to a bug in
NJOY 89.31 and has been removed already by R.E. MacFarlane in NJOY 89.62 version.

e. Interpolation law for total cross section

For some isotopes (see Fig. 14 for $^{14}$N and Fig. 15 for Si), the line shapes calculated by
RECENT and RECONR did not agree for the total cross section in the lower energy region. The
reason is that RECENT reconstructs the total cross section respecting the interpolation law
specified for the total in the basic file, while the RECONR module of NJOY defines the total
to be the exact sum of the reconstructed partials. The conclusion is that the interpolation law
for total cross section in ENDF/B-VI is inadequate for such cases. More examples and
discussions on this point are found elsewhere [13].

f. The 'artifacts' in comparison plots

There are 'artificial' discrepancies due to a convention of RECENT using repeated energy points and NJOY not using this convention at the boundary of resonance region. RECENT interprets the data on the two sides of the boundary as two completely different types of data which need not be continuous at the boundary. It seems unlikely that these differences could significantly affect calculations of integrals in the two systems.

g. Concluding remarks on the IAEA code verification project

The potential users of ENDF/B processing codes should be aware of possible errors that can arise in their processing of ENDF/B library.

NJOY is designed for long word-length computers and as such the readers should be aware of the approximations involved in using NJOY on short word-length machines.

Reactor physics teams working on different reactor concepts around the world using NJOY or RECENT (either recent or earlier version) will be interested to see the comparison plots obtained for many materials in this intercomparison study, apart from alerting the user that the accuracy of data processing cannot be taken for granted for all isotopes, in all energy regions, and for all reactions.

This section also distinguishes between differences due to the codes themselves and differences due to inconsistencies in the basic ENDF/B-VI evaluations- for example, as was pointed out in the text of this report, the differences in the unresolved region and in the definition of the total cross section are due to inconsistencies in the basic evaluations which have allowed NJOY and RECENT to each interpret the data in a non-unique way leading to different results- the method to eliminate these differences should not focus only on having NJOY and RECENT do exactly the same thing (which authors of NJOY and RECENT can agree to do) but focus on clarifying and documenting the ENDF/B conventions and procedures so that any other code will also calculate the same results.

4. WIMS LIBRARY UPDATE PROJECT

The International Atomic Energy Agency has initiated a project to update the multigroup nuclear data input library of the WIMS reactor physics code (in short: WIMS Library Update Project). The WIMS code is one of the most widely used thermal reactor physics codes and is of interest especially to reactor physics groups in developing countries. The WIMS Library Update project is principally conceived to proceed through a series of thermal reactor benchmark calculations using the evaluated nuclear data libraries, nuclear data processing codes and the WIMS code, with a gradual replacement of old by new nuclear data, and, including at

152
each step, a checking of the reliability of the calculational results. Deviations between calculated and experimental benchmark data will be used to remedy inaccuracies in the calculations and/or nuclear data input and will also be fed back to the originators of the codes and/or evaluated nuclear data for review and improvement. The final outcome of this project will thus be a reliable up-to-date nuclear data base for the WIMS code in its present 69 energy groups format for all materials based on the newly released basic evaluated data files. Project participants in particular those from the developing countries will acquire a detailed knowledge of nuclear data relevant to thermal reactor physics as well as a capability for reliable use of an important reactor physics computer code and associated nuclear data processing codes. M. Ravnik and A. Trkov from the Josef Stefan Institute in Ljubljana, Slovenia are responsible for the technical coordination of this project. The status reports for the first two stages have been written [19,20]. One of the authors (S. Ganesan) is in charge of this project at the Agency. The project is being carried out primarily through correspondence and at no cost to the Agency.

The processing part of WLU project involves the use of available processing codes including NJOY and several related and interesting code developments. For instance, the non-availability of a WIMSR module prior to NJOY 91.0 has led some teams to develop their own post-processors (e.g., WIMSLIC developed in Korea [21]) to post-process the output of POWR module of NJOY. Care should be taken to obtain consistency between the options used in NJOY and the post-processor to the definitions of group constants as needed by the WIMS code. The details of this project and the current status are outlined by M. Ravnik and A. Trkov at this meeting in their presentation.

5. TRAINING ACTIVITIES ON NJOY

An in-house group fellowship training on nuclear data processing and reactor applications was organized at the IAEA Nuclear Data Section by the Agency during the period March - June 1991 in which six IAEA fellows successfully participated: The training program, which was conducted by D.W Muir and S. Ganesan and the staff of Nuclear Data Section, involved the following IAEA Fellows:

1. Fortunato AGUILAR HERNANDEZ (Mexico)
2. Vesselin LALEV (Bulgaria)
3. Abderrahmane MALKI (Algeria)
4. Muhammad ARSHAD (Pakistan)
5. Shafiquil Islam BHUIYAN (Bangladesh)
6. Riyanto RAJARDO (Indonesia)

The training program consisted of several informal lectures on ENDF/B formats and procedures, physical meaning of the input options used in NJOY for the generation of PENDF and GENDF files and practical computer exercises using the NJOY system. The version NJOY 89.31 was extensively used during that period by the Fellows to obtain experience in the use of NJOY to generate PENDF and GENDF files from ENDF/B-VI and JENDL-3 files for a few selected isotopes. A preliminary generation of 69 group constants in WIMS format was also
attempted with some success for some light isotopes. It is planned to continue this training activity on NJOY in the future, depending on the level of interest from the developing countries and the availability of funds. One of the future activities of the Agency in the area of nuclear data processing will be to provide selected PENDF and GENDF files produced as a result of these training activities for free distribution to those who are interested to post-process such files to suit their specific application requirements. Such in-house fellowship training on NJOY is recognized as very useful to scientists even if they are interested to undertake only post-processing in their countries, where the resources are limited in terms of computer resources and manpower to undertake a complete NJOY computation starting from the basic evaluated data file.

REFERENCES

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13. S. Ganesan and D.W. Muir, "First Results of Intercomparison of NJOY 89.31 with the IAEA pre-processing codes for FENDL materials for zero Kelvin and 300 Kelvin Cross section Line Shapes of ENDF/B-VI," IAEA Nuclear data Section, Unpublished, May 1991.


Fig. 1
Fig. 2
Fig. 6

N16O ENDF/B-VI (RECENT)
N16O ENDF/B-VI (NJOY)
-14.9 to 99.8% Differences

N16O ENDF/B-VI (NJOY) / N16O ENDF/B-VI (RECENT)
Fig. 7

NI60 ENDF/B-VI (RECENT) / NI60 ENDF/B-VI (NJJOY)

Cross Sections

-30.6 to 42.1 Z Differences

NI60 ENDF/B-VI (RECENT)

NI60 ENDF/B-VI (NJJOY)
Cross Sections

Fig. 8

$10^{-1}$

1.10
1.05
1.00
0.95
0.90
0.85

1.00166 1.00168 1.00170 1.00172 1.00174

KeV

Recent

Ratio
Fig. 12
Fig. 14

Cross Sections

N14A ENDF/B-VI (RECENT)
N14A ENDF/B-VI (NJOY)

10^2
10^1
10^0

1.00
0.96
0.92
0.88

10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^0 10^1

Ratio
Fig. 15

Total Cross Sections

S100 ENDF/B-VI (RECENT) -3.97 to 0.379% Differences
S100 ENDF/B-VI (INJOY)

Ratio

MeV

10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^0 10^1
NJOY-91 and Thermal Reactor Applications

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Abstract

NJOY91.13 data processing code is being installed on the VAX computers at the Institute "Jožef Stefan". This version of NJOY has a new WIMSR module which links the evaluated data files to the WIMS group constants library for thermal reactor applications.

At the International Atomic Energy Agency (IAEA) a WIMS Library Update Project is in progress. It is based on international participation from a large number of laboratories. The main stages of the project serve to standardise WIMS inputs for modelling benchmark experiments, to check the data processing codes and procedures and to update the WIMS library with more recent data.

Stage 1 which included 5 benchmark lattices has been completed recently. Preliminary results of Stage 2 have been analysed. They include the results from the South Korean WIMSKR module of NJOY87. It is planned to include the results of NJOY91 before proceeding to the next stage.
1 Introduction

NJ0Y91.13 has recently been received from RSIC and is in the process of installation on one of the VAX computers at the Institute "Jožef Stefan" (IJS). During installation some trivial programming inconsistencies were encountered: character constants of different lengths were transferred to subroutines where they were declared as fixed length character strings. Due to this inconsistency they were incorrectly interpreted on VAX.

Compared to the previous versions of NJ0Y, the installation procedure on VAX is much simpler since fewer operations are required to adapt the machine-dependent parts of the source code. Unfortunately the installation could not be completed due to an error on the transmittal tape which corrupted a number of statements in the CONVER routine in the source code. In the test cases 3 and 5 which were completed, differences in excess of 1% were noted in the numerical results. Their physical significance was not investigated in further.

For thermal applications the main extension of NJ0Y91 compared to previous versions is the addition of the WIMSR module. There exist some local interface modules which link the evaluated data files with the WIMS library through older versions of NJ0Y (such as prepared in Canada, Switzerland and South Korea, for example). These are non-standard modules and are limited by compatibility to a particular version of the NJ0Y code. With NJ0Y91 a standardised version of the WIMSR module has been released, which will eliminate most of the compatibility problems in the future.

The WIMS library, which is supplied with the non-commercial WIMS-D4 code is based on very old data, adjusted to obtain better agreement with the measurements on the so-called benchmark experiment lattices. The overall agreement of the results with this library is not bad, but it is felt that an improvement is possible by updating the library with data from one of the most recent evaluated data files.

2 WIMS Library Update Project

The WIMS Library Update Project (WLUP) was initiated through the International Atomic Energy Agency (IAEA) in August 1990 when an invitation letter [1] was sent to several potential participants in different laboratories throughout the world. The main stages of the project serve the following purposes:

1. standardisation of WIMS inputs to model benchmark experiments,

2. checking the data processing codes and procedures by data intercomparison,

3. updating the WIMS library with more recent data for some important reactor materials,

4. supplementing the updated library with the remaining materials of interest (including fission products).

Stage 1 had been completed recently [2] and is hoped to be extended to include more benchmark experiments. Preliminary results of Stage 2 had been analysed [3]. A summary of results is presented in the sections below.
2.1 Standardisation of WIMS inputs for benchmark experiments

Five benchmark test cases [4] were specified (TRX-1 and 2, BAPL-1, 2 and 3). Participants were invited to provide the main benchmark results which were given in the benchmark specifications, together with basic software and hardware specifications: the code and the library version, the type of computer.

The possibility of WIMS/D4 code installation errors was eliminated by comparing the results for a model input, which was identical for all participants and provided by the project coordinators. The standard WIMS library supplied with the WIMS/D4 code distributed through the NEA Data Bank was used in the exercise.

First contributions arrived in November 1990, most of them arrived by February 1991, while several late participants sent their contributions as late as October 1991. Altogether, 23 contributions have been received.

The results of the benchmarks were filed and tabulated. The definition of the integral parameters which are compared to the measured values are given in Table 1.

<table>
<thead>
<tr>
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</thead>
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<tr>
<td>$k_{\infty}$</td>
<td>infinite medium multiplication factor,</td>
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<tr>
<td>$k_{\text{eff}}$</td>
<td>finite medium effective multiplication factor,</td>
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<tr>
<td>$\rho^{28}$</td>
<td>ratio of epithermal to thermal $^{238}U$ capture,</td>
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<td>$\delta^{25}$</td>
<td>ratio of epithermal to thermal $^{235}U$ fission,</td>
</tr>
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<td>$\delta^{28}$</td>
<td>ratio of $^{238}U$ fission to $^{235}U$ fission,</td>
</tr>
<tr>
<td>$C^*$</td>
<td>ratio of $^{238}U$ capture to $^{235}U$ fission.</td>
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</tbody>
</table>

A preliminary evaluation was performed. Some trivial errors were removed either by repeating the calculations or by contacting the participants. The average values of the calculated parameters and their standard deviation (labelled RELDEV) of the results provided by the participants are presented in Table 3. The reference results calculated using the standardised inputs and their difference from measured values (labelled RELDIF) are also given. The following conclusions may be drawn about the results:

- Significant differences in $k_{\text{eff}}$ can be observed between the results of different participants. The distribution of $k_{\text{eff}}$ is presented in graphical form in Figure 1. Each bar in a diagram corresponds to the number of participants with $k_{\text{eff}}$ results in the $j^{th}$ interval $[k_{\text{eff}}^{(j-1)}, k_{\text{eff}}^{(j)}]$ of width $\Delta k$ which is arbitrarily chosen as 0.1% of the average $k_{\text{eff}}$. The spread of the results is mainly due to different input models. It is bigger than the differences due to the modifications of the code, which are practically negligible. The spread of the results shows properties of the normal distribution, what indicates that the differences arise more due to uncorrelated effects than to biases or systematic discrepancies.

- The peaks of the distributions of $k_{\text{eff}}$ in Figure 1 correspond closely with the most sophisticated (but still practical) input models which may be used in WIMS (using a large number of groups, $S_n$ order greater than default, $B_1$
approximation). These inputs are declared as standard and will be used in the subsequent stages of the project. The results obtained with such inputs may be defined as reference when making conclusions about the agreement of the calculations and the measurements. They are given in Table 3 (labelled REF.) and they are marked with an arrow in Figure 1. They agree well with the average results calculated by the participants.

- It may be observed that the reference results lie at the limit (or just outside) of the error interval (dotted line in Figure 1) for $k_{eff}$. A systematic shift of the reference $k_{eff}$ results may be observed if all benchmark cases are compared. WIMS $k_{eff}$ is overestimated for TRX-1 and BAPL-1 which are both rather tight lattices compared to TRX-2 and BAPL-3, where $k_{eff}$ is underestimated. The dependence of the error in $k_{eff}$ on lattice pitch or fuel/water ratio either stems from the resonance calculation method in WIMS (Dancoff corrections), methods for the effective diffusion constant and leakage calculations or from the cross sections which are used in this calculations. The effect is relatively strong (total shift of 0.6% $\delta k$ between TRX-1 and TRX-2 or 0.55% $\delta k$ between BAPL-1 and BAPL-3). According to the sensitivity analysis calculations the effect is too strong to be attributed to the WIMS calculational models alone. The sensitivity analysis and references [4] suggest that the error in $k_{eff}$ can be better explained by the error in the resonance integrals of U-238. This is also in agreement with the observed errors in the calculated spectral indicators (particularly $\rho^{28}$) which are discussed below.

- The influence of different input options is not so strong in the case of other benchmark parameters ($\rho^{28}, \delta^{25}, C^*$), as they depend only on the spectrum and on the particular isotope microscopic cross-sections. The spread of the results reflected in the standard deviations in Table 3 is relatively small. It may be observed that the calculated results systematically lie within the experimental error interval for $\delta^{25}$ and $\delta^{28}$ while for $\rho^{28}$ and $C^*$ they are mainly out of it.

Parameter $\rho^{28}$ is underestimated by approximately 4% in the case of TRX-1 and 2 and by approximately 2% in the case of BAPL-1 and 3. In the case of BAPL-2 the overestimation of $\rho^{28}$ is small. Experimental value for $C^*$ is provided only for TRX-1 and 2, in both cases the calculated $C^*$ being approximately 2% underestimated. Both results indicate that the epithermal capture of U-238 is underestimated by about 4%. Independently, from the good agreement for $\delta^{25}$ and $\delta^{28}$ it can be concluded, that the U-235 fission reaction rate in the denominator of $C^*$ being correct, the U-238 capture is responsible for the discrepancies. Since $\rho^{28} \approx 1$, the thermal and the epithermal capture are approximately equal. Assuming that the thermal capture is correct, the error in $C^*$ should be two times smaller than that of $\rho^{28}$, as it is indeed observed.

- The WIMS $\rho^{28}$ is on average underestimated, indicating that the resonance cross-sections are probably underestimated, yielding overestimated $k_{eff}$ in tight lattices, where the spectrum is harder and $\rho^{28}$ is large. Going to lattices with a bigger lattice pitch (such as TRX-2 or BAPL-3), $\rho^{28}$ becomes smaller and
the error in the resonance integral becomes less important. The $k_{ef}f$ is less overestimated, i.e., it is shifted in the negative directions with respect to the experimental value.

The conclusion that the epithermal and the resonance capture cross sections in WIMS U-238 data are incorrect can not be definitely confirmed but it is consistent with the observed indications, although there are also many other unaccounted effects which may influence the results. Among them it is important to note that the epithermal capture of U-238 is underestimated also due to the definition of the U-238 absorption cross section in the WIMS library, which is modified to preserve neutron balance on account of multiple neutron emission reactions such as $(n,2n)$.

2.2 WIMS library data intercomparison

2.2.1 Objectives

The calculated parameters of Phase 1 results contain errors due to errors in the nuclear data as well as errors due to inadequate physical models in representing the actual experimental configurations. To some extent these two sources of error can be decoupled by repeating the calculations using a cross section library (such as ENDF/B-IV), the performance of which is well known from the literature. By comparing the calculated results to the published data, the error contributions from the physical models and the multigroup constants library format limitations can be distinguished from the errors in the data (assuming that the data processing errors are small). Furthermore, the choice of the ENDF/B-IV library for code verification purposes broadens the selection of the participating codes since practically all of them can process ENDF-4 formatted data but not ENDF-6. The main objectives of Stage 2 of the project are the following:

- by comparing the data calculated by different processing codes, check for data processing errors, and errors in the group constants definitions (if possible),

- since the WIMS library format restrictions prohibit exact data representation for general cases, optimize the assumptions and processing routes in preparing the WIMS library by investigating their effect on global lattice parameters,

- by comparing the WIMS results (using ENDF/B-IV based library) to published results for the same benchmark lattices (particularly the results of more sophisticated calculational methods), establish the WIMS modelling capability for the selected benchmarks.

2.2.2 Data processing

The participants on the project were asked to process hydrogen bound in water, oxygen, aluminium, uranium-235 and uranium-238 from the ENDF/B-IV evaluated nuclear data library, under the same conditions as in the original WIMS library (particularly with regards to temperatures and background cross section values for the cross sections and resonance integrals tabulations). Five sets of results were
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<tr>
<td>IAP</td>
<td>Institute of Atomic Physics, Bucharest, Roumania</td>
<td>various</td>
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<tr>
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<td>Institute &quot;Jožef Stefan&quot;, Ljubljana, Slovenia</td>
<td>FEDGROUP-C86 (Rev.3)</td>
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<td>Korean Atomic Energy Research Institute, Choong-Nam, Republic of Korea</td>
<td>NJOY/87</td>
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Cross sections and resonance integrals (for uranium isotopes) were compared. Burnup chains (if specified) and other data were not checked at this stage. Scattering matrices were also not checked in detail.

A reference data set for comparison was established using processing codes [5] LINEAR, RECENT, SIGMA1, GROUPIE which are reliable and extensively tested [6,7,8]. All cross sections were Doppler broadened to 300K. The averaging function was the Maxwellian-1/E-Fission spectrum, similar to the one used in most of the other processing codes. The selected set of codes is not ideal because it can not produce all the data types required. The definition of the resonance integrals also differs from the one assumed in WIMS. Nevertheless, it provides an independent data set to which all other data can be compared. A small modification to the GROUPIE code was made such that the resonance integrals as required in WIMS could be calculated assuming that the product of the Goldstein-Cohen parameter λ with the potential cross section σp in the resolved resonance range was constant.

In Figure 2 an example of cross section intercomparison is presented. The difference in the transport cross section of $^{238}U$ between IJS and reference data arises due to the IJS assumption that the scattering cross section is fully shielded (approximated by the potential cross section). The differences between the NJOY results and reference in the fast energy range are due to the differences in the averaging spectrum.

In Figure 3 an example of the resonance integrals intercomparison is presented. Fairly good agreement in the absorption resonance integrals as a function of the background cross section is observed at lower energies (except at very high levels of self-shielding). At higher energies a discrepancy is noted between the reference GROUPIE data (obtained with a fixed value of $λσ_p$) and the IJS and NRI results which use the Intermediate Resonance approximation. GROUPIE and NJOY results calculated with purely Narrow Resonance approximation agree with each other but differ strongly from other results.
2.3 Conclusions

The analysis of the WIMS results contributed by different laboratories for modelling the benchmark experiments inspires confidence, that the standardised inputs are appropriate for modelling the selected benchmarks. It has been proposed that an extension to Stage 1 should be carried out to include more benchmark experiments that can be modelled with WIMS.

Detailed intercomparison of group averaged cross sections inserted into the WIMS library through various independent processing routes indicates, that differences which could be attributed to data processing errors are quite small, particularly for the codes which participated in the Code Verification Project [6]. Most of the discrepancies could be traced to some differences in the definitions, or to data processing assumptions due to format limitations of the WIMS library.

Some open questions regarding the definition of the resonance integrals remain to be answered, particularly the relation between the resonance integrals and the self-shielded cross sections. The integral effects of the approximations in the calculation of the resonance integrals also requires some further investigation.

In view of the results presented so far it would seem appropriate to include the NJ0Y91 results in the analysis before finalising Stage 2. This would provide a contribution to the verification of the WIMS module of NJ0Y which is new and it would simplify processing of new evaluated data libraries which could not be processed by some other codes due to format limitations.

References

[1] Letter from Dr. S. Ganesan, IAEA, to participants of WLUP project, 334-F4.01, dated 27. August 1990,


Table 3: Averages of values calculated by participants and reference results

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Figure 1: Distribution of calculated $k_{eff}$ values for the benchmark lattices
Figure 2: Transport cross section comparison of Uranium-238 for IJS and KAERI data.
Figure 3: Background dependence of the absorption resonance integrals of Uranium-238 in Groups 23 and 27.
Processing EFF-2.2 with ACER of NJOY 91.13
to produce an MCNP library

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Via E.Fermi, 27 00044 Frascati(ROMA)
April 1992

Abstract
In the frame of the Fusion Technology Programme of the European Community a task was
promoted to supply the NET Team with evaluated data especially oriented to shielding needs, then
at the same time, to supply the NET with a working library for neutron and photon calculations. The
task of ENEA-Frascati was to produce a working library for the Monte Carlo code MCNP which we,
at the moment, have in the latest distributed version 4.2. At the porpuse, the processing NJOY
system was used, installed on a 3090 IBM computing machine. Previously the evaluated library
EFF-1 distributed in the summer 1988, was processed\textsuperscript{3,4} using NJOY 87.1. The library has been
used for many kinds of neutronical calculations\textsuperscript{3,6}. This work now relates on the processing of the
EFF-2.2 library, further step of the EFF project, distributed in late 1991 in ENDFB-VI format, by
means of NJOY 91.13.

Details on processing with NJOY
The derived library from EFF-2.2 is a standard portable 80 bytes per record library in a
special format, ACE (A Compact ENDF), which is suitable by MCNP. The processing work has been
undertaken by means of NJOY 91.13 system ACER is the final processing module used.
With the latest version 91.13 we solved many of the previous problems\textsuperscript{7,8} concerning
precision. At Frascati ENEA NJOY is installed on an IBM 3090-300 machine (single precision: 32-
bits per word) when originally it is written for a Cray machine (double precision: 64-bits per word).
Installing NJOY on a different machine, like an IBM, is not immediate, it can give problems mainly
related to the reduced default precision\textsuperscript{9}. Following suggestions of people working at Winfrith
(UKAEA)\textsuperscript{10}, a double precision NJOY system was successfully implemented on IBM. The latest
library for MCNP from EFF-2.2 has been derived by means of this version.
The NJOY chain used is: MODER, RECONR, BROADR, HEATR and ACER.
MODER is used just to convert ENDF tapes from the EBCDIC formatted mode to blocked-
binary for a faster data flow through the chain.
RECONR is used to reconstruct cross-sections from ENDF/B scheme to a linear interpolation
scheme within a specified tolerance. A reconstruction at 0\(\textsuperscript{o}\)K, with a tolerance of .5% and 7
significant digits, has been adopted.
Then data have been Doppler-broadened to 300\(\textsuperscript{o}\) K with a subsequent thinning (similar to
RECONR) by means of BROADR module.
HEATR has been used to calculate and add to the output tape the local neutron heating (MT
301). This then is put in the ESZ block with total, elastic and capture cross section on the output ACE
file. Heating calculation is based on an energy balance method. The problem with this method is that,
modest errors in the photon or neutron emission tables, can lead to negative values. On the other
hand, the excess photon energy can be repositioned elsewhere in the system. The result is that we can
have errors in the heat distribution in the system. Others\textsuperscript{11}, in case of negative neutron heating
values, prefer to use the upper kinematic limit (MT 443), which, nevertheless, could be a conservative estimate. HEATR can be used also to calculate the energy available for damage (MT 444), to be output in dosimetry files. We used this capability in MCNP dpa rate calculations for Fe, Ni, Cr and Cu (for EFF-1 library only at the moment).

ACER is the module specifically written to prepare a data library for the Los Alamos continuous energy Monte Carlo code MCNP. The integral thinning option with infinite dilution ($\sigma_0 = \infty$) was used, trying to reduce the input energy points (a maximum 8000 number of energy points were asked) keeping the total and capture integral cross sections to 0.5% of their original value. In the new NJOY release (91.13), ACER needed few changes for a correct run. In subroutine CHANGE a wrong instruction made pointers and data starting from the LD/LW block to be incorrect. In the same way a too low value of variable TESTE in subroutine ACELOD, made photon data processing from MF13 to be not consistent with the GPD block (total photon production cross section). Then running MCNP, a failure in sampling photons with proper MT, was recorded. The TESTE value was then changed to process all the photon data subsections in MF13. Still there are problems in processing some of the EFF-2.2 materials (see table 1). Sometimes in MF5 more than 2 interpolation regions for a given MT are given, leading to a stop in subroutine CPTAB; also for MF6 no format is accepted other than the Kalbach-Mann. The solution could be or a change in the input data or maybe a deeper change in ACER, or in MCNP itself.

Index to EFF-2.2 library

In table 1 elements from EFF-2.2 contained in the MCNP library EFF22 are shown together with their identification number ZAID. Till now only one of the 3 sublibraries of which EFF-2.2 is made of (tape 200) was processed. It contains data for materials not evaluated within the EFF-2 programme but which were selected from recent released libraries (JEFF-2, ENDFB-VI and JENDL-3). Their origin with few comments about the contained data and processing are given as well. In table 2 the dictionary used by MCNP to read the ACE EFF22 library is given. Work is in progress in comparing these new evaluations with previous ones from the other libraries distributed with the code MCNP.

References

2) H. Gruppe laar: "Status of the European Fusion File" ECN Petten, EFF-DOC-17 July 1988
3) L. Petrizzi: "NJOY modules...to produce an ACE library from EFF-1 for ... MCNP" Seminar on NJOY-THEMIS June 1989 NDB, OECD Saclay, France
4) L. Petrizzi: "EFF-1 Data processing for MCNP" May 1990, EFF Meeting Saclay, France
6) V. Rado, L. Petrizzi, M. Gallina: "3-D shielding analysis of the magnet in the ITER system" contract n° NET/90-240, final report Sept. 91.
### Table 1

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### Table 2

**MCNP dictionary for EFF-2.2**

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185
Session 4:

USER EXPERIENCE AND
PROGRAM MAINTENANCE

Chair:
Doug Muir
ANALYSIS OF NEUTRON DEEP PENETRATION EXPERIMENT
BY TRIPOLI CODE

S.H. ZHENG

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CENTRE D'ÉTUDES NUCLEAIRES DE SACLAY
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A neutron deep penetration benchmark experiment has been carried out at AEE Winfrith to provide information of benchmark quality for the test of data and of calculation method. The neutron spectra over the range 50KeV to 5MeV have been obtained and the activation of a range of threshold has been measured. This benchmark is interpreted by the Monte Carlo code TRIPOLI in multi-group model with the neutron cross sections based on UKNDL and ENDF/B4 libraries; the influence, on the results, of the numbers of energy groups and the cross sections processing method is analyzed.

Introduction

In this study, the AEE Winfrith iron neutron deep penetration experiment(I) has been analyzed by the Monte Carlo code TRIPOLI(2) in the multigroup model to validate the calculation method and the iron cross sections in UKNDL (United Kingdom Nuclear Data Library) and ENDF/B4 (United States Evaluated Nuclear Data File) libraries. The multigroup cross sections are generated by the nuclear data processing systems NJOY and THEMIS(3-4) using ENDF/B4 library, and by the system LINDA(a) using UKNDL library.

A low power natural uranium converter plate, driven by the source reactor NESTOR provided a large thin disc source of fission neutrons at the interface of a graphite moderator and a extensive iron shield.

The converter plate consisted of a fissile section of 50.8 cm square by 3.18 mm thick; the total power of the converter plate is 7.26x10^4±5% watt per Nestor Watt at which power the fission rate at the centre of the converter plate was 3.346x10^3±5% fission/(sec cm Nestor Watt), the spatial distribution of the fission rate in the converter plate in a cosine function of width 142.9 cm and the equivalent area disc has a radius of 59.3 cm.

\[
f(r)=3.346\nu_{25} \cos(\pi r/142.9)\pm5%
\]

(neutron/sec/cm^2/Nestor Watt)

The neutron spectrum of the source is represented by the uranium 235 fission spectrum,

\[X(E)=0.453 \exp(-1.0123E) \sinh\sqrt{2.1893E}\]

The iron shield consisted of 24 mild steel plates each 180x191cm^2 and 5.08 cm thick, there is a 6.35 mm air gap between adjacent plates to allow to detect the detectors.

The chemical components of the iron shield and the others parts of the experiment are given in the table 1 (the region number corresponds to the number in the figure 1).

Three detectors are used to measure the neutron reaction rates, RhiO3(n,n')RhiO3m, In 115(n,n')In 115m and S32(n,p)P32, all results of the measure are given in 10^8 d.p.s. per Nestor Watt; the estimated standard deviation of each detector is (6):

Rh: ±3%
In: ±2%
S: ±4%
**Calculational geometry**

In the calculation, the R-Z two-dimensional geometry proposed by McCracken(2) was used, all rectangular components of the experiment are represented by cylinders of equal base area, the air gaps between adjacent iron plates were replaced by iron and the atomic density of the iron shield was reduced by the factor \(50.8/(50.8+6.35)\), the geometry of the calculation is showed in the figure 1.

**Neutron cross section**

The UKNDL neutron data is used to study the influence of the numbers of energy groups, the multigroup average cross sections a-re generated by the LINDA system without considering the self-shielding.

The NJOY and THEMIS systems are used for treating the neutron multigroup cross sections from ENDF/B4 library, for energies above 1MeV, the cross section is weighted by the fission spectrum; below 1MeV, the \(I(E-S\Sigma)\) factor is used to weight the cross section, where \(\Sigma\) is the total cross section of the composition; for iron, two general compositions are considered (mild steel and stainless steel); the thermal energy range is not important in this calculation.

**Monte Carlo techniques**

The Boltzmann equation is solved in TRIPOLI code by using the Monte Carlo method in three-dimensional geometries; for deep penetration calculation, the biasing techniques are necessary to reduce the variance on the results with a reasonable computer time. For this object, the free-path biasing is defined as exponential transforme, the collision biasing, the splitting and the Russian roulette are also used to reduce the variance. The source biasing is very important for a fast neutron calculation (e.g. the reaction rates of Rh103, In115 and Sp1 in this case the neutron source with high energy is very important), if it is not a great part of the uranium 235 fission source. The figure 2 shows the natural and the biased neutron sources in the calculation.

**Results and discussion**

With UKNDL library, two multigroup models are used to obtain the results (310 groups and 6000 groups in which the numbers of groups above 1MeV are 57 and 3400). The calculations results are compared with experiment results in the figure 3, the neutron spectra are given in the figure 4.

From the results, following items are pointed out:

1. At small distance, the results of the two calculations are not very different because the self-shielding effect is not important;
2. At great distance, the self-shielding effect become very important, if the multi-group cross sections were not weighted by a self-shielding factor, the results would be very sensitive to the numbers of energy groups.

In the calculation with ENDF/B4 in 315 groups, the multigroup cross sections are weighted by a self-shielding factor (fission spectrum or \(I(E-)\)); it has given the better results than the UKNDL 310 groups calculation for the detectors Rh103 and In15 (the resonances region) at great distance. The results and the spectra are showed in the figures 3 and 4.

**References**

2. J.C. Nimal et coll., "Programme de Monte-Carlo poly-cinetique a trois dimensions TRIPOLI-02".
Fig. 1 Calculational geometry of the benchmark ASPIS
1, 3, 7: Aluminium  2: Carbon,  4, 6: Air,  5: Converter plate,
8: Iron shield,  9, 12: Mild steel,  10, 11: Concrete.

Figure 2  The neutron natural and biased source.
Figure 3  Comparison of the calculation results and the experiment results
C1: Calculation UKNDL 310 groups;  C2: Calculation ENDF/B-IV 315 groups;
C3: Calculation UKNDL 6000 groups;  E: experiment.
(a). detector Rh103(n,n')Rh103m;  (b). detector In115(n,n')In115m;
(c). detector S32(n,p)P32.
Figure 4  The comparison of the neutron spectra between the calculations and the experiment. 
(a). distance d=57.15 cm;  (b). distance d=114.3 cm.

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(*) Density reduced to allow for air gaps.
HEAVY NUCLEUS RESONANCE ABSORPTION IN AN HETEROGENEOUS LATTICE

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Why do we use code comparisons?

The calculation of the space and energy dependence of the heavy resonance absorption in an heterogeneous lattice is one of the hardest work in reactor physics. The APOLLO 2 (ref 1) code uses a self shielding formalism to compute the spatial and energetic dependence of the self shielding. As there is no clean experience to isolate and qualify this phenomenon, we have to use code comparisons. There are two very fine calculation codes used to validate the Apollo 2 results:

- TRIPOLI: (ref 2) performs accurate Monte Carlo calculations, with a pointwise representation of the cross sections in the resonance range.
- SECOL: (ref 3) performs a very fine resolution of the slowing down equation, using a 10,000 group averaged library.

Test case:
The code comparisons and the validation is only possible because we use the same evaluation for the three codes APOLLO 2, TRIPOLI and SECOL, and the same processing code, THEMIS/NJOY (ref 4, 5).
The geometry chosen is a very simple one: an infinite fuel pin, containing one strongly resoning isotope (U8, Pu240, Th232,...), surrounded with a clad and placed in water as moderator.

Results:
For one neutron slowed down below 1.51 keV, we compare the absorption rate of the heavy nucleus between 1.51 keV and 3 eV or in the low thermal part for Pu240, for the different energy groups and the different regions of the pin. The results have been reported by Mr Henry Tellier and Miss Coste in the following reference: "heavy nucleus resonant absorption calculation benchmarks", presented in the Charleston conference, 1992.

REFERENCES


4 - "THEMIS: Sytème de traitement des sections efficaces - presentation - manuel d'utilisation" C. M. Diop, D. Chaigne, G. Dejonghe, J. Gonnord, M. J. de Villeneuve, CEA internal report.

PLUTONIUM 240 ABSORPTION
172 groups-Background matrix
Peripheral area
\[ \Delta p = (\pm 37 \pm 30) \times 10^{-5} \]
THORIUM 232 ABSORPTION
172 groups-Background Matrix
$\Delta \rho=\left(-100\pm84\right)\times10^{-5}$
USE OF NJOY/THEMIS SYSTEM IN THE SCOPE OF THE SENSITIVITY, UNCERTAINTY AND DATA ADJUSTMENT ANALYSIS

I. KODELI

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A code system devoted to the sensitivity, uncertainty, and adjustment analysis has been developed at CEA Saclay. The computational scheme implemented is presented in Figure 1. Various sensitivity and uncertainty analysis (e.g. due to the uncertainties in the cross sections, response functions, spectrum and space distribution of neutron source, expansion to Legendre polynomials) can be performed, as well as the adjustment of the basic data to experimental results. The package was applied to the 900 MWe EDF power plants with the objective to validate the methodology used in the pressure vessel surveillance programme /2/, as well as to the ASPIS benchmark experiment, and similar procedures found their application in the fusion calculations.

In the scope of this package NJOY/THEMIS modules occupy a central role. In particular they are used to perform the following tasks:

- The partial cross-sections are required in SUSD /3/ code to calculate the sensitivity profiles. They are expected in a groupwise ENDF (GENDF) format. GROUPR module of NJOY is therefore used to produce self-shielded multigroup cross sections and anisotropic scattering matrices for the reactions of interest.

- Up to now only ENDF/B-4 based cross section libraries like VITAMIN-C, SAILOR were used for transport calculations. In future with the NJOY/TRANSX compatibility problems fixed, GENDF files will be further processed via MATXSR module of NJOY and TRANSX code /4/ to prepare the problem dependent group cross-section library based on ENDF/B-6 data. The cross section library for transport codes and the partial cross sections for SUSD will be thus produced in a completely consistent way.

199
A module to be linked to the NJOY/THEMIS system is under development to introduce the modifications suggested by adjustment, to the nuclear cross section data in the PENDF file, in particular to the iron elastic and non-elastic cross sections.

The covariance data are taken from VITAMIN-J/COVA /5/ covariance data library, written in BOXER format and the program ANGELO is used to extrapolate/interpolate these data to the user group structure (see Figure 2). Output of ANGELO can be either in binary form or in COVFILS format as used in the ERRORM module of NJOY. If written in COVFILS format these data can be further processed using the COVR module of NJOY for the graphical presentation of multigroup covariance data, or to write them in the compact BOXER format. Graphical presentation offers a possibility of inspecting the reasonableness and formal correctness of the original covariance data as well as of the interpolation scheme.

ANGELO group collapsing procedure was in addition validated by comparison to the procedure implemented in NJOY/COVR module. Good correspondence was found between the two (Figure 3), and ANGELO: COVR module was adopted mainly because of the practical reasons (user friendly handling, great flexibility due to the variety of the input data formats allowed).

NJOY/COVR module is used to produce new covariance matrices in BOXER format, as required by ANGELO, from the recent data like ENDF/B-6.

References


Figure 1: Code system used for the sensitivity, uncertainty and adjustment analysis.

Figure 2: Data flow scheme of the procedure in VITAMIN-J/COVA library.
Figure 3: Comparison of the covariance matrices obtained using the codes NJOY and ANGELO. The covariance matrices are practically identical, although contrary to NJOY no flux weighting is used in ANGELO.

Note also the unrealistic reduction of uncertainties near threshold which indicates that NJOY group collapsing strategy in this region should be verified.
I. Introduction

This paper describes briefly the work that has been required for treating a EFF library to generate a TRIPOLI Monte Carlo code library for fusion studies.

II. EFF-1 file

The European Fusion File (EFF-1) is a neutron cross-section file for application in fusion reactor field [3].

The contents of EFF-1 are given in details in references [3] and [4]. EFF-1 file contains the following non-fissile isotopes:

H, D, T, Li6, Li7, Be, B10, B11, C, Al, Si, Ti, V, Cr, Mn, Fe, Ni, Cu, Zr, Nb, Mo, Ba, W, Pb, Bi.

Cross-sections of these materials are stored in ENDF/BV standard format except for the continuum inelastic (MT = 91), (n,2n) (MT = 16) and (n,3n) (MT = 17) reactions on Lead and (n, 2n) reaction on Beryllium. Both cases will be examined in the next section.
III. Processing for building a TRIPOLI library

3.1 - Processing Scheme

The scheme of the neutron cross-section processing is shown in Figure 1. For neutron transport calculations the TRIPOLI-2 code [1] requires one of the following two types of cross-section library: a punctual cross-section library or a multigroup cross-section library. Figure 1 concerns the building of a multigroup cross-section library, by using the THEMIS/NJOY system of codes [5]. The number of energy groups is 318; this multigroup structure is given in Annexe I. Nevertheless, in a TRIPOLI-Library, anisotropy is described in an energy punctual mode: it is the aim of ANISO module which computes cosinus, \( \mu_i(E) \), of equiprobable intervals from the PENDF file (MF = 4) (see Figure 1):

\[
\int_0^{\mu_i+1(E)} f(E,\mu) \, d\mu = \frac{1}{N},
\]

\( f(E,\mu) \) being the neutron scattering law on file MF = 4.

For TRIPOLI-2 library: \( N = 32 \).

The continuum inelastic scattering is assumed isotropic in the Center of Mass.

3.2 - Treated Materials

Materials actually treated are the following:

H, D, T, Li6, Li7, Be, B10, B11, C, Al, Si, V, Cr, Fe, Ni, Zr, Nb, Mo, W, Pb.

The precision criterium for cross-section reconstruction is ERR = 0.005 and broadening temperature: 300 K.
3.3 - The Specific Processing Scheme for Lead

In EFF-1, files 4 and 5 do not exist for Lead, but the energy-angle distributions (double differential cross-sections) are given on file 6 in ENDF/BVI format for continuum inelastic (MT = 91), (n,2n) (MT = 16) and (n,3n) (MT = 17) cross-sections.

In order to build a TRIPOLI-2 cross-section library with our present processing codes, it is necessary to have standard ENDF files 4 and 5 in ENDF/B format. Therefore, we used the GROUPXS module [6], to convert file 6 in standard ENDF/BV files 4 and 5. A new BCD lead file has been created from the initial BCD file, by inserting the new files 4 and 5 obtained by the GROUPXS module, and by suppressing the non-standard file 6. Dictionary and sequence numbers have been updated. It is evident that in this operation, we loss the energy-angle correlations.

The following formula gives the definition of the quantity stored on file 6 in EFF-1 and those stored on files 4 and 5 (cf reference [6] p.12 to 14):

- double differential cross-section : \((E, E' = \text{energy, } \Omega, \mu = \text{angle})\)

\[
\frac{d^2\sigma(E' - E', \Omega)}{dE' \ d\Omega} = \frac{\sigma(E) y(E)}{2\pi} f_0(E' - E') b(E' - E', \mu)
\]

where:
- \(\sigma(E)\) = scattering cross-section versus energy
- \(y(E)\) = neutron yield
- \(f_0(E' - E')\) = energetic law transfer
- \(b(E' - E', \mu)\) = energy-angle normalized distribution.

We have:

\[
\int_{-1}^{+1} b(E' - E, \mu) d\mu = 1
\]

and the Legendre Polynomial \((P_1(\mu))\) decomposition:

\[
f_0(E' - E') b(\mu, E' - E') = \sum_{l=0}^{1} \frac{2l+1}{2} f_1(E' - E') P_1(\mu)
\]

205
Then:

- File 6 contains $E'$, $f_0(E-E')$, $b(\mu, E-E')$: double differential cross-section
- File 5 contains $f_0(E-E')$: energetic transfers
- File 4 contains $C_1(E) = \int_{0}^{E_{max}} f_1(E-E')dE'$: anisotropy of reaction in accordance with the standard ENDF/B5 format [7].

### 3.4 - The (n,2n) Reaction on Beryllium

This reaction can be developed as it follows:

$$\text{Be}^9+n \rightarrow \text{Be}^{9+}+n' \rightarrow \text{Be}^8+n \rightarrow 2\alpha.$$ 

In the EFF-1 file, the (n,2n) reaction is described as a discrete inelastic scattering $(n,n')$ (from $MT = 51$ to $MT = 83$ levels in ENDF/B format).

Such a description requires to multiply the neutron weight by a factor 2 when the (n,2n) on Be9 is chosen during the TRIPOLI simulation. This operation assumes that the energetic emission laws of both neutrons are independent.

### 3.5 - The Weighting Spectrum to Compute Multigroup Cross-Sections

Multigroup cross-sections are weighted by a spectrum $\phi(E)$ which depends on the energy range:

- For $E > 12.523$ MeV, $f(E) = \frac{1}{a \sqrt{\pi}} \exp \left[ -\frac{E - <E>}{a} \right]$
  
  $a = \frac{2}{m_n} kT <E>$  \hspace{1cm} $<E> = 14.07$ MeV
  
  $kT = 25$ KeV
  
  $a = 0.53199$ MeV

- For $0.41399$ eV $< E < 12.523$ MeV

  $f(E) = \frac{C_1}{E}$  \hspace{1cm} $C_1 = 2.82334 \times 10^{-3}$
For $E < 0.41399$ eV

$$f(E) = C_2(T) \exp \left( - \frac{E}{kT} \right) \quad T = 300 \text{ K}, \ kT = 0.026 \text{ eV},$$

$$C_2(300) = 1.3549 \times 10^5$$

This weighting option has been implemented in the GROUPN module of NJOY/Themis system [5].

IV. Examples of TRIPOLI calculations with EFF-1 library


- A three dimensional calculation of neutron streaming through ITER tokamak pumping ducts with the Monte Carlo code TRIPOLI-2, in Fusion Engineering and Design 18 (1991) 377-385, I. Bresard, C. M. Diop, L. Giancarli, F. Gervaise

![Diagram of EFF-1 processing system](image)

Figure 1: Processing of neutron cross-section library EFF-1 fusion file for TRIPOLI Monte Carlo code

207
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NJOY TO DETECT IMPROPERLY DEFINED DATA

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Abstract

NJOY has been used to verify some parts of SIXPAK/1, a code for checking all double differential data (MF = 6) and to output in equivalent MF = 4, MF = 5 and MF = 15 data. In this paper one point deduced from the analysis of the results that could be of interest both for code developers and for data evaluators is highlighted.

Introduction

The ENDF/B double differential (correlated) data in MF = 6 represent data in the form:

\[ \sigma(E,E',\cos\theta) = \sigma(E) \times \gamma(E) \times g_0(E,E') \times f(E,E',\cos\theta) \]

where:

- \( \sigma(E) \) \hspace{1cm} MF = 3 cross section
- \( \gamma(E) \) \hspace{1cm} yield (multiplicity)
- \( g_0(E,E') \) \hspace{1cm} energy spectrum
- \( f(E,E',\cos\theta) \) \hspace{1cm} angular distribution

with the conditions:

\[ \int f(E,E',\cos\theta) d\cos\theta = 1 \]

and:

\[ \int g_0(E, E') \int f(E,E',\cos\theta) d\cos\theta dE' = 1 \]

The format for MF = 6 data is described in /2/ in which all parameters, flags and quantities are properly defined. In particular we wish to outline:

- \( g_0(E,E') \) is given in /2/ as \( g_0 \);
- \( f(E,E',\cos\theta) \) can be given given both in parametric (Legendre coefficients or Kalbach-Mann systematics) and tabular form depending on the two parameters LAW and LANG.

SIXPAK performs the following checks on MF = 6 data:

\[ ^1 \text{Presented at the April, 1992 NJOY Meeting, NEA Data Bank, Saclay (Paris).} \]
Parameters

All parameters are checked for consistency. If parameters are not consistent the program may not be able to perform the following tests and will merely skip a section of data.

Interpolation laws

All interpolation laws are checked. All data associated with interpolation laws are checked, e.g., no non-negative values requiring log interpolation. In order to perform required integrals over \( \cos \theta \) and \( E' \) it is imperative that the interpolation laws be compatible with the data.

All integrations are performed using the interpolation law.

Spectra and angular distributions

All spectra and angular distributions are checked to insure they are normalized and do not include any negative values.

Legendre coefficients

The normalization, \( f_o \), cannot be negative.

Legendre coefficients are checked in the range -1 to +1.

Angular distributions are checked at \( \cos = -1, 0 \) and +1.

Furthermore SIXPAK, by integrating \( f(E, E', \cos \theta) \) over \( E' \) and \( \cos \theta \) produces uncorrelated angle and energy distributions to be put in MF = 4 and MF = 5, respectively. Also MF = 15 photon spectra are generated.

An NJOY application

Before processing a large number of materials for building group libraries, it is worthwhile to perform checks with any tools at disposal, i.e. standard and/or not standard checking codes, in order to avoid loss of man/computer time. With SIXPAK, unusual features have been found in one material in which the MF = 6 data are defined by the following parameters:

- LCT = 1 laboratory data for both angle and secondary energy;
- LAW = 1 continuum Energy-Angle distribution;
- LANG = 12 tabulated angular distributions to be interpolated linearly.

The code reported:

- non constant energy dependent yield for \((n, 2n)\) reaction;
- some boundary angular distributions normalized to 0 instead of 1.

In fact the yield shows the following shape: 0 at the threshold (about 8.3 MeV), 2 from 8 to 20 MeV while it must be 2 in the whole range for the \((n, 2n)\) reaction and the angular distributions have all zero probability at most part of \( E' \) for which \( g_\sigma(E, E') \) is zero, i.e. at the boundaries of the spectra.
Those assumptions possibly come from the fact that where the spectrum \(g_\nu(E, E')\) is zero the evaluator also set the yield \(y(E)\) and angular distribution \(f(E, E', \cos \theta)\) to zero - which can lead to some very strange effects when one interpolates between energies.

Some examples of these strange effects:

1. the yield is 0 at 8.3 MeV, increases to 2 at 8.5 MeV and is then constant up to 20 MeV. This means between 8.3 and 8.5 MeV the number of neutrons emitted will vary from 0 to 2;

2. because of the completely zero angular distributions at the lower and upper energy limits of the spectra, for energies near these points the \((n, 2n)\) emission will be depressed;

3. again in the energy range 8.3 to 8.5 MeV the yield is varying from 0 to 2, the spectrum starts at 0 and increases and the angular distribution starts at 0 and increases to isotropic at 8.5 MeV. This means at 8.4 MeV the yield is 1, the angular distribution will integrate to 1/2 (instead of 1) and the spectrum will be 1/2 its value at 8.5 MeV. If the spectrum is assumed correct then the \((n, 2n)\) emission at 8.4 MeV will be only 1/4 what it should be - 1/2 from the yield and 1/2 from the angular distribution.

We fix the data as follows:

1. the yield at 8.3 MeV should be 2, not 0;

2. the angular distributions at the lower and upper energy limits should be the same as at the nearest energy point - at the lower energy limit usually isotropic, but at the upper energy limit usually allowing only extremely forward or backward emission.

In order to have a visual measurement of the effects of the above modifications, the original and the modified data have been first processed by NJOY 89.62 into the 175 energy group VITAMIN-J structure to obtain the \((n, 2n)\) transfer matrix and the results have been plotted comparing all outgoing groups from each group of incident energy from the two sources.

The comparison (carried over with COMPLIT /3/) shows big differences in the shape of the groups generated from the 20-th incident energy group (8.18 to 8.6 MeV) which contains the threshold (graph no.1) and minor effects in the other incident energy groups (the remaining graphs), where the boundary groups only have different values and the original data are lower than the new ones accordingly to the modifications; also the sum of the outgoing groups is lower for the threshold group (the last graph).

Further developments

We intend in the future to verify the results of the transfer matrices obtained by NJOY using MF=6 and MF=4+MF=5, which should be exactly the same for the zero-th order; what is lost is the correlation between \(E'\) and \(\cos \theta\), however, in many applications where there is a broad spectrum of neutrons and the neutron flux is not highly directionally oriented, the neutron multiplication, spectrum and orientation can be fairly accurately calculated without considering correlation effects. An important consideration is that many computer codes - data processing and transport codes - cannot use the correlated (MF=6) data - nor are they intended for high energy use. For these codes the uncorrelated data produced by SIXPAK should be adequate to meet their needs.
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