Recent Progress On NJOY

by

Robert E. MacFarlane
Nuclear Theory and Applications Group
Los Alamos National Laboratory

ABSTRACT

The NJOY nuclear data processing system is used all over the world, and it has been selected as the standard processing code for the European nuclear data effort. These comments have been prepared for the December 1996 meeting of the European NJOY Users' Group, being held at the NEA Data Bank in Paris in conjunction with the JEF/EFF meeting, which coordinates the European efforts to create a common file of data for nuclear applications.

I. INTRODUCTION

The NJOY nuclear data processing system is used to transform evaluated nuclear data in the ENDF (evaluated nuclear data files) format into forms useful for nuclear application calculations. Because of the favorable convergence of nuclear data formats all over the world, these evaluated data can come from the US ENDF/B libraries, the European JEF libraries, the Russian BROND libraries, the Japanese JENDL libraries, the Chinese CENDL libraries, the IAEA FENDL libraries, and others.

NJOY has become fairly stable over the last couple of years. Changes are being driven by the wide variations between evaluation techniques in the many ENDF-format libraries, by the exposure to more users and more kinds of computers, by the ever increasing demands of users for convenience and comprehensiveness, and by the ongoing projects to extend nuclear data files to higher energies for accelerator applications. Some of the new features encouraged by these trends include the gas-production capability, a DPA capability for MCNP, a radionuclide production capability, extensions for high-energy angular distributions and KERMA factors, and color graphics.

II. GAS PRODUCTION

The isotopes of hydrogen and helium generated as byproducts of nuclear reactions (either emitted particles or residuals) can be important in evaluating material damage, or they can even be the ultimate product of the machine (*e.g.,* tritium in a fusion reactor blanket). This "gas production" is implicit in the reaction cross sections included in a nuclear data evaluation, but it is much more convenient for the user if the gas-production cross sections are separately tabulated in the application libraries. The ENDF-6 format has a set of reaction identifiers, or "MT numbers," already defined for this purpose, namely, MT=201–207 for ^{1}H, ^{2}H, ^{3}H, ^{3}He, and ^{4}He, respectively. However, only a few evaluations contain data in these sections.

In the past, gas-production values have sometimes been constructed from other data available in the application files; for example, by using TRANSX edit commands to construct a response function for multigroup codes. Also the ENDF/B-V version of the data files for the MCNP Monte Carlo code contains gas-production cross sections added directly to the ACE file. However, we decided that it would be more flexible to define a new module for NJOY that could compute the gas cross sections from the basic reactions and add them to the PENDF tape using MT=201–207. This is parallel to the procedure used to add other information (such as KERMA, damage, and thermal scattering), and it makes consistent cross sections available for subsequent plotting, multigroup processing, or Monte Carlo formatting.

The new module is called GASPR, and it was turned on with updates up11, up13, and up14. It knows about the emitted particles and residual nuclei produced for all the standard ENDF MT numbers. It also can use the LR flags given in the files to define how the residual nucleus can break up; for example, MT56/LR22 for oxygen is the reaction (n,n$_6$)α ^{13}C. An even more complicated problem occurs for high-energy evaluations that use File 6 with MT=5—the particle yields can be energy-dependent fractional numbers. The module prints a summary table that shows how each gas-production cross section was assembled from the reactions given in the evaluation.

Once the gas-production cross sections have been written onto the PENDF file, they can be group averaged just like any other reaction. The MATXSR module has been modified to read these group-averaged results from the GENDF tape and put them into reactions on the MATXS library. The names chosen for the gas reactions have the form ".h1" or ".he3". Actually, "nxh1" and "nxhe3" might have been better—the names beginning with dots have to be given with delimiters in the TRANSX input file. The ACER module has also been modified to make use of the gas-production data. It automatically plots its cross sections as part of our Quality Assurance procedure, and Figures 1 and 2 show examples of the results.

GASPR has been included in many of our processing runs. The results are included in the FENDL Monte Carlo and multigroup libraries designed for use on the ITER fusion-reactor project, and many gas-production curves are available on line through *http://t2.lanl.gov/*.

III. DPA For MCNP

Radiation damage due to atomic displacement is important for commericial power reactors (*e.g.,* pressure vessel damage), but it is especially critical for fusion reactor designs because of the very high fluences of high-energy neutrons expected. Because of the economic penalties associated with frequent change outs of important components, accurate prediction of material damage is critical. NJOY has long had the capability to compute "damage-energy production" in the HEATR module and pass it through GROUPR for multigroup applications. However, these numbers weren't previously available for use in Monte Carlo codes like MCNP in a convenient way. Starting with up19, we have modified the ACER module to take the existing damage cross sections (MT=444 on the PENDF tape) and include them on the ACE library file. Following the MCNP tradition, they are given in units of MeV-barns. The phenomenological treatment of radiation damage assumes that a certain "displacement energy" is required to create a particle-vacancy pair, and that the available energy is consumed in making these pairs. An efficiency factor is also normally used. Therefore, the displacements per atom (DPA) cross section is given by

$$\mathrm{DPA} = \eta \frac{\sigma_\mathrm{d}}{2E_\mathrm{d}} \tag{1}$$

The displacement energies vary from about 25 to 90 eV. A table of typical values is given in the HEATR chapter of the NJOY report. A typical efficiency value is 80%. It is up to the MCNP user to apply these two factors during the construction of a DPA tally.

Damage-energy production cross sections have been generated for many of the ACE files, and the results can be viewed at *http://t2/lanl/gov/* in the Data area. An example is shown in Figure 3.

IV. RADIONUCLIDE PRODUCTION

Another problem that is characteristic of fusion-reactor analysis is computing the portion of the steady-state heating that is due to the decay of short-lived radionuclides. The prompt component of the heating has long been available from the HEATR module of NJOY, either processed through GROUPR for the MATXS files, or converted directly into ACE format for MCNP.

It has been argued that a good estimate for the decay portion of the heating can be obtained by summing up the energy release from radioactive nuclei with decay times up to 1 day. Longer lived nuclei are important for waste considerations, but they do not appreciable affect the heating during steady-state operation. The local heating due to beta decay or conversion and the corresponding gamma lines are well known. They can be supplied to TRANSX for multigroup calculations using files like delay12 and delay24, which are included in the TRANSX distribution. However, it is also necessary to know the rate of production of each of the radionuclides being used. For reactions in isotopic evaluations, these rates are just equal to the reaction cross sections, which are included in full detail in MATXS libraries. An example of some lines from delay42 for an isotopic target follows:

```
  1 np 1.101e6  mn55  / mn55(np)cr55 (3.5m)
  1 nh 1.005e6  mn55  / mn55(nhe3)v53 (1.6s)
-23 nh .90      mn55  /    1.006
-23 nh .10      mn55  /    1.289
  1 na 1.069e6  mn55  / mn55(na)v52 (3.8m)
-22 na .00588   mn55  /    1.3336
-21 na 1.       mn55  /    1.434
-21 na .00116   mn55  /    1.531
  1 ng .8310e6  mn55  / mn55(ng)mn56 (2.6h)
-24 ng 1.0      mn55  /     .84675
-19 ng .275     mn55  /    1.8107
-18 ng .145     mn55  /    2.1130
-17 ng .010     mn55  /    2.5229
-17 ng .0066    mn55  /    2.6574
-17 ng .0031    mn55  /    2.9598
```

The lines starting with “1” add the local decay heating to the KERMA in position 1 of the transport table. The lines beginning with negative numbers insert a gamma ray into the appropriate part of the gamma production area of the transport table. The reaction cross section used is just (n,p), (n,^{3}He), or (n,α)

However, many evaluations are for elemental targets. In these cases, it is necessary to supplement the evaluation with production cross sections for the radionuclides. Unfortunately, there is no standard way to do this. We decided to make use of the MF8/9/10 mechanism of the ENDF format, which is really intended for isomer production cross sections for a particular isotope. With a few small extension, it is quite suitable for giving production yields or cross sections for different nuclides (and isomers) for an element. This capability was added to GROUPR and MATXSR using up11 and up12. So far, we have only worked on radionuclide heating in a multigroup context, and MCNP is not supported. GROUPR is told to process the radionuclide cross sections using and input card of the form "10/". It automatically loops over all the necessary reactions. MATXSR inserts the cross sections into a normal vector data record using names of the forms "r13126" or "c25056". The first name denotes the production of the ^{26}Al* isomer, and the second represents the production of ^{56}Mn by capture. The "c" will be used in a future version of TRANSX to trigger a self-shielding treatment. With these cross sections available, a TRANSX run using edit lines like the following will produce a steady-state transport table for an elemental target:

```
  1 r22045 .3742e6 tinat / tinat(nx)ti45 (3.08h)
-28 r22045 2.0     tinat /   .511
  1 c22051 8.68e5  tinat / tinat(nx)ti51 (5.76m)
-31 c22051 .93     tinat /   .320
-26 c22051 .0118   tinat /   .609
-24 c22051 .069    tinat /   .929
  1 r21146 .0537e6 tinat / tinat(nx)sc46m (18.7s)
-34 r21146 1.0     tinat /   .1424 it
  1 r21048 .2270e6 tinat / tinat(nx)sc48 (43.7h)
-24 r21048 1.0     tinat /   .9835
-23 r21048 1.0     tinat /  1.3121
-23 r21048 .976    tinat /  1.0376
-33 r21048 .0748   tinat /   .1754
-23 r21048 .0238   tinat /  1.2129
  1 r21049 .8176e6 tinat / tinat(nx)sc49 (57.2m)
  1 r21050 1.648e6 tinat / tinat(nx)sc50 (102.5s)
-20 r21050 1.0     tinat /  1.5538
-23 r21050 .995    tinat /  1.1211
-27 r21050 .887    tinat /   .5238
  1 r21044 .5972e6 tinat / tinat(nx)sc44 (3.93h)
-28 r21044 2.0     tinat /   .511
-23 r21044 1.0     tinat /  1.1570
```

This new decay heating treatment is now being made available in the FENDL-1 library for use in ITER fusion-reactor design calculations.

V. HIGH-ENERGY ANGULAR DISTRIBUTIONS

As the energy of the incident particle increases, angular distributions for two-body reactions like elastic and inelastic scattering get more and more forward peaked. The ENDF system has always had an official limit to the Legendre order of 20. This is certainly sufficient for the original ENDF energy limit of 15 MeV, but it suffers some at 20 MeV, and it is totally inadequate for the energies of 150 MeV being used in new evaluations for accelerator applications.

It has been argued in the past that using the Legendre representation with more than 20 terms is inappropriate, that tabulated values should be used instead. However, optical model theorists in our Group and elsewhere feel that expansions as high as order 64 are quite well founded using modern optical-model codes. Even when tabulated distributions are used in the evaluations, NJOY still has to be able to work internally with Legendre expansions of order commensurate with the forward-peaking in the tabulated distributions. This is true in both HEATR and GROUPR. Therefore, we have begun the process of extending the code to use expansion up to order 64. The HEATR module has been upgraded and tested on some recent high-energy evaluations that used tabulated distributions for energies up to 150 MeV. GROUPR will be upgraded in future updates.

It should also be noted that the same representation (tabulated or Legendre expansion) must be used at all incident energies. Thus, when a high-energy extension is added to an existing evaluation, the angular distributions below 20 MeV have to be converted to tabular form. This is inconvenient, does damage to the evaluator's intent, and is inefficient.

As a result of this work, we decided to ask the Cross Section Evaluation Working Group (CSEWG) to approve an extension of the ENDF-6 format that allows up to order 64 for Legendre expansions. This request was approved at the November 1996 meeting.

The MCNP Monte Carlo code uses 32 equally probable cosine bins for each incident energy to represent angular scattering. If the backward cosine is always -1.0 (as in all current sets), but most of the distribution is concentrated near cosines of 1.0, 3the scattering will be into back angles where there is very little actual scattering possible. This problem can be alleviated by allowing the backward limit to be some value higher than -1.0. We are experimenting with a patch that detects cases where the integral from -1.0 to mu is very small and chooses a new backward limit such that this integral is less than `aback`=1.e-4. A larger value might be preferable for this limit. Tests on several materials show that this change in the backward limit only shows up for incident energies greater than 20 MeV.

In the long range, it might be better to abandon the equally probable bins and use a cummulative distribution function to sample angular distributions in MCNP. This would be consistent with the approach used for energy distributions.

VI. HIGH-ENERGY KERMA

The heating produced by a flux of particles in a material is important for many reasons. It may have to be removed by a heat transfer system, it may lead to local melting or damage, or it may cause a superconducting magnet to transition to normal conductivity. This last is a case where one wants to reduce heating by careful shielding. The KERMA is also a key quantity for medical radiotherapy calculations, but in this case, one may want to design to enhance heating in critical regions of the body. All such calculations require the best possible data on nuclear heating in convenient forms for applied calculations.

For ENDF/B-V-type evaluations, we have been able to use the HEATR module of NJOY to estimate the KERMA from the cross sections and distributions given in the file. This was always a difficult process because of energy-balance faults in the evaluations and the difficulty of getting good numbers as small differences between larger quantities. The plague of negative KERMA values is still endemic in all the evaluated data libraries. More recently, File 6 became available, giving evaluators a capability to put recoil energy-angle distributions in directly. Where this capability has been used, it has significantly improved the representation of both KERMA and damage (the Oak Ridge evaluations for the iron group, copper, and lead are good examples).

The use of File 6 puts the burden of calculating recoil spectra on the evaluator (where it belongs), but these calculations begin to become very difficult as energies increase and multiple reaction channels open up. Comprehensive calculations, such as the one used in the RECOIL code for analyzing nuclear model calculations done with GNASH, become prohibative for energies above 30 or 40 MeV. Mark Chadwick has recently revisited this problem in the context of step-wise preequilibrium reactions.

The energy-angle distributions of emitted particles can be represented well and compactly using Kalbach systematics in the center-of-mass frame of the original collision; however, things are more complicated for the recoil nuclei. The backward kick from primary particle emission in the CM tends to make the recoils look a little more isotropic in the lab frame. But the representation of the angle and energy of the recoil emissions in the CM would be very complex and bulky. In practice, it is really only the energy spectrum in the lab that is needed for most applications (*e.g.,* heating and damage). Therefore, Chadwick developed methods to estimate the recoil spectra from the multistep reaction process in the laboratory frame. We have proposed a format modification to CSEWG called "LCT=3." LCT is the flag that is set to 1 for using the lab frame and to 2 for the CM frame. Our proposal says that when LCT=3, the primary particle emissions are given in the CM frame, but the recoil spectra are given in the lab frame. This proposal has been implemented in NJOY, and it was accepted at the November 1996 CSEWG meeting. Our group has prepared several new evaluations for energies extending to 150 MeV, and they all use this new format. Figure 4 shows several of the KERMA curves to 150 MeV from this work.

VII. COLOR GRAPHICS

Whether you think of color as a necessity, a user convenience, or a wastfull frill, NJOY now has it! The first step was to extend the VIEWR module to be able to fill backgrounds and draw curves in color. Since Postscript fully supports color, this wasn't too difficult. It was difficult to choose a scheme. We decided to use a restricted model with limited capabilities for the user. For 2-D plots, curves are represented using a limited set of dark colors. The region inside the graph frame and the page background around the graph frame can be chosen from a set of light pastel colors. Text (except for curve labels or tags) is always given in black. For 3-D plots, one light pastel color is used for the page background, and another is used to fill the polygons representing each member of the family of curves. The curves, axes, and labels are always black. Figures 5 and 6 are examples of the 2-D and 3-D plots that can be made with NJOY's new color capability.

The VIEWR and PLOTR input instructions have been modified slightly to be more compatible. This makes it easier to edit VIEWR input into PLOTR decks when necessary. They both support the same variables for specifying colors. They both now support a capability for filled areas. Areas can be filled with one of the background colors, with one of a set of colors designed to show contours (similar to the shades of greens or blues used for mountains or oceans on maps), or with a pattern of hatching or cross-hatching lines.

As a consequence of these input changes, it was also necessary to modify the VIEWR outputs from HEATR, DTFR, and ACER to match. These three modules still produce black-and-white graphs by default. But the COVR module has been modified to take advantage of the new ability to make color contour graphs. Figure 7 is a demonstration of color covariance plotting.

VIII. FUTURE WORK

One of the first priorities will be upgrading PURR, ACER, and the formats for MCNP to support the use of probability tables for unresolved-resonance self shielding. An experimental capability for this has been available for many years. Now, it will finally be packaged and incorporated into the standard, supported versions of MCNP.

In another project resulting from our high-energy work, we will be upgrading ACER and the data formats for MCNP to support libraries for incident charged particles (especially protons), including full representations of secondary charged particles in each library.

We will continue to receive and review patches and suggested new capabilities contributed by NJOY users.

It is about time for a new major version of NJOY. One feature that might be included is a new configuration management scheme that would make updating NJOY more automatic. This scheme would also enforce a level of automatic documentation that would help to satisfy the requirements of Quality Assurance programs.

FIGURE CAPTIONS

Figure 1. An example of gas production cross sections as produced by the new GASPR module and printed out during the ACE QA procedure.

Figure 2. Another example of gas production cross sections from GASPR, this one showing its capability to work at energies up to 150 MeV by computing the contributions from MF=6 and MT=5.

Figure 3. An example of a damage energy production cross section from an MCNP data library file. The ACER plotting package also shows this cross section as a log-log plot to emphasize the low-energy region.

Figure 4. Examples of high-energy KERMA curves as produced from the new 150 MeV evaluations with the "LCT=3" option.

Figure 5. A typical NJOY 2-D plot using the new color capability of the PLOTR and VIEWR modules.

Figure 6. An example of a 3-D plot with color added.

Figure 7. The capability of the new color plotting additions to fill regions with ranges of colors can be used to good effect for showing the covariance matrix as a contour plot. In previous plots of this type, hatching and cross-hatching with varied line spacing had to be used to identify the difference levels of covariances.