Nuclear Criticality Safety Engineer Training
Module 13 [1]

Measurement and Development of Cross Section Sets

LESSON OBJECTIVES

1) Explain the steps involved in creating a cross section set for use in criticality safety calculations, including the techniques used to measure cross section data, process the data, evaluate the dataset, and release the evaluated nuclear data file (ENDF) for use in computer codes.

2) Provide general guidelines for selecting the correct code and cross section set for various problems.

INTRODUCTION

Most criticality safety analyses today utilize Monte Carlo methods. Results of these calculations depend on the cross section libraries used by the codes. That is, deficiencies in their nuclear data libraries are translated into deficiencies in the results of the Monte Carlo calculations that predict criticality or k_{eff} for measured critical experiments or for proposed operations with neutron multiplying materials.

Deficiencies in the performance of a criticality safety method, e.g., a Monte Carlo code/data library package, are determined by validation, i.e., calculations of a series of benchmarked critical experiments. This data testing process may indicate discrepancies in the nuclear data for a specific nuclide and reaction, such as fission in ^{233}U or scattering in Pb, and may suggest the need to update or reevaluate the nuclear data for that nuclide. This new evaluation might be based solely on existing differential cross section measurements, but in some cases this reexamination of the available data might suggest the need for new measurements. Additional cross section data might be needed 1) to eliminate discrepancies in the existing measured data, 2) to obtain measured data in an energy range in which data are not currently available, or 3) to reduce the uncertainty in the evaluated cross sections. This evaluation process might also use nuclear theory model codes to obtain the best fit or shape of the new evaluated cross section data. This new evaluation may be proposed to be adopted by the cross section evaluation working group (CSEWG) and become part of the official ENDF/B files. These new evaluated cross section data can then be processed into the data libraries used by the criticality safety codes.

This training module will describe how neutron cross section measurements are performed and how the data are evaluated and tested, then ultimately introduced into the ENDF/B libraries to contribute to the improvement of criticality predictions. The flow diagram showing how nuclear

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[1] Developed for the U.S. Department of Energy Nuclear Criticality Safety Program by Eric C. Howell, Purdue University, in conjunction with Oak Ridge National Laboratory and the DOE Criticality Safety Support Group.

cross section data are provided to support nuclear applications in the U.S. is presented in Figure 1. Typically, nuclear data measurements are performed at cross section measurement facilities such as the Oak Ridge Electron Linear Accelerator (ORELA), Los Alamos Neutron Science Center (LANSCE), etc. Subsequently, nuclear physics tools are used to perform data analyses to prepare evaluated cross section data files for dissemination in the ENDF/B file system. Before the evaluated cross section data can be used in radiation transport analyses, cross section processing software (i.e., AMPX, NJOY, PREPRO, etc.) is used to process the ENDF/B files and prepare cross section libraries for use with radiation transport software (i.e., SCALE, MCNP, VIM, etc.). The transport software along with the processed data libraries can be used to model nuclear systems to calculate integral quantities of interest. As shown in Figure 1, the performance of the nuclear data and radiation transport software for the application of interest or benchmark problems can identify the need for improved nuclear data. As needed, the nuclear data deficiencies can be addressed by performing new nuclear data measurements and/or cross section evaluations. In the first part of the training module, an overview is provided for the tasks that are needed to perform nuclear data measurements and analyses to prepare cross section data files for the ENDF/B file system. The training module concludes with a brief overview of cross section data preparation tasks for supporting radiation transport analyses.

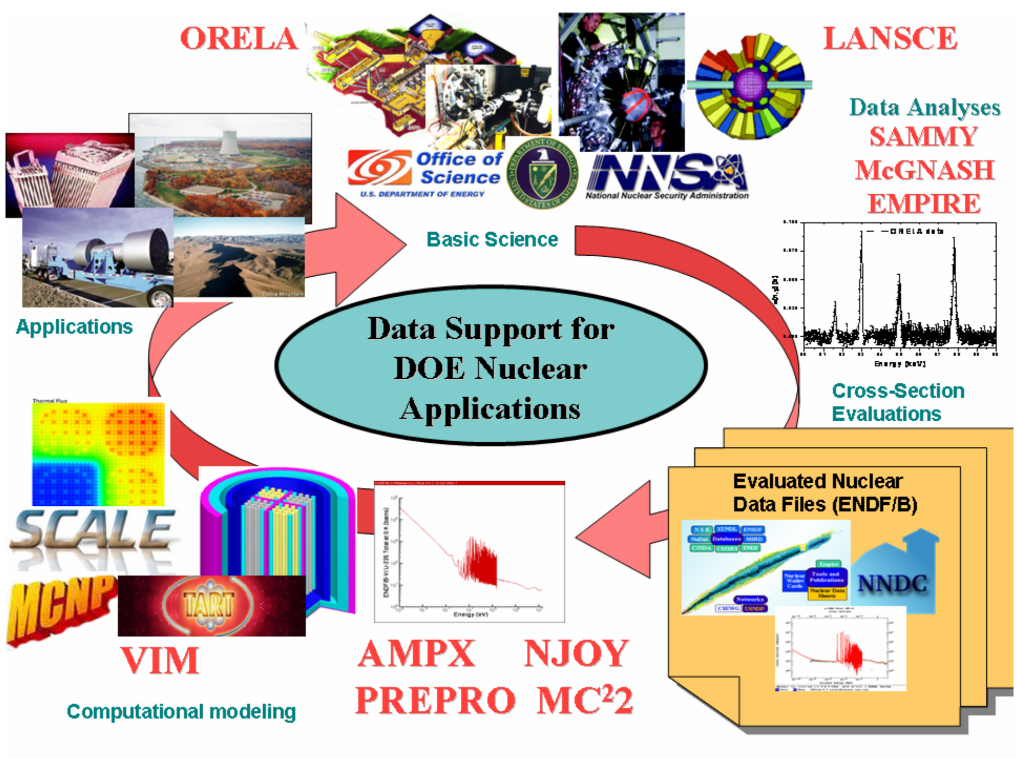

Figure 1. Nuclear Data Flow Diagram for Supporting Nuclear Applications

NEUTRON MEASUREMENTS

The fact that neutrons are electrically neutral is the main complication in the measurement of neutron-nucleus reaction cross sections. In measurements with electrons and protons, electric and magnetic fields can be used to accelerate, filter, focus, bunch, and detect the particles directly. For neutrons, ingenious systems that take advantage of the nuclear properties of various materials must be utilized.

Neutron Sources

The first problem that needs to be addressed is the production of neutrons. Both the quantity and the energy spectrum of the neutrons are important. Large numbers of neutrons are required to reduce statistical errors associated with the measurement of reaction cross sections. Detailed knowledge of the neutron energy spectrum is required to determine energy dependent cross sections. Two common sources of neutrons are nuclear reactors and sub-critical piles. The main advantage of these sources is that they produce large neutron fluxes. Initial measurements of reaction cross sections were made with these devices by oscillating a sample into and out of the core. Each oscillation would cause a pulse in the reactivity of the system. By measuring the pulse amplitude and comparing it to the pulse of a sample with a known cross section one can calculate an integral cross section. However, such cross sections are an average over one particular neutron spectrum and as such they can only be used in systems with a similar spectrum. Considering the broad range of applications today, from reactor design to spent fuel processing and storage and criticality safety, simple integral cross sections are no longer technically acceptable for most analyses.

Other sources of neutrons include white sources, with neutron energies from sub-thermal up to several hundred MeV, isotopic sources (e.g., ^{252}Cf) and mono-energetic sources. In a white neutron source, a target with high atomic number, e.g., tungsten, is bombarded by highly energetic charged particles. In the case of high energy protons the neutron production process is called spallation whereas with high energy electrons photons are produced which in turn produce the neutrons via (γ,n) reactions. Examples of spallation neutron sources are the SNS (Spallation Neutron Source) at Oak Ridge National Laboratory (ORNL), LANSCE at Los Alamos National Laboratory (LANL), IPNS (Intense Pulsed Neutron Source) at Argonne National Laboratory (ANL), and the neutron time-of-flight (n_TOF) facility at CERN (Conseil Européen pour la Recherche Nucléaire). Electron driven neutron sources are ORELA (Oak Ridge Electron Linear Accelerator) at ORNL**,** RPI (Rensselaer Polytechnic Institute) Gaerttner LINAC (linear accelerator), and the GELINA facility at the Institute for Reference Materials and Measurements (IRMM). Increasing the energy of the incident particle increases the number of neutrons emitted. Figure 2 shows the typical neutron flux spectra of some white sources. Table 1 gives an overview of the parameters of the various neutron sources. One disadvantage of white neutron sources is that they also create large doses of gamma radiation as a byproduct as well as other high energy particles, therefore heavy shielding is sometimes required. Currently, several facilities in the U.S. perform neutron induced cross section measurements, i.e. LANSCE at LANL, IPNS at ANL, ORELA at ORNL**,** and the Gaerttner LINAC at RPI.

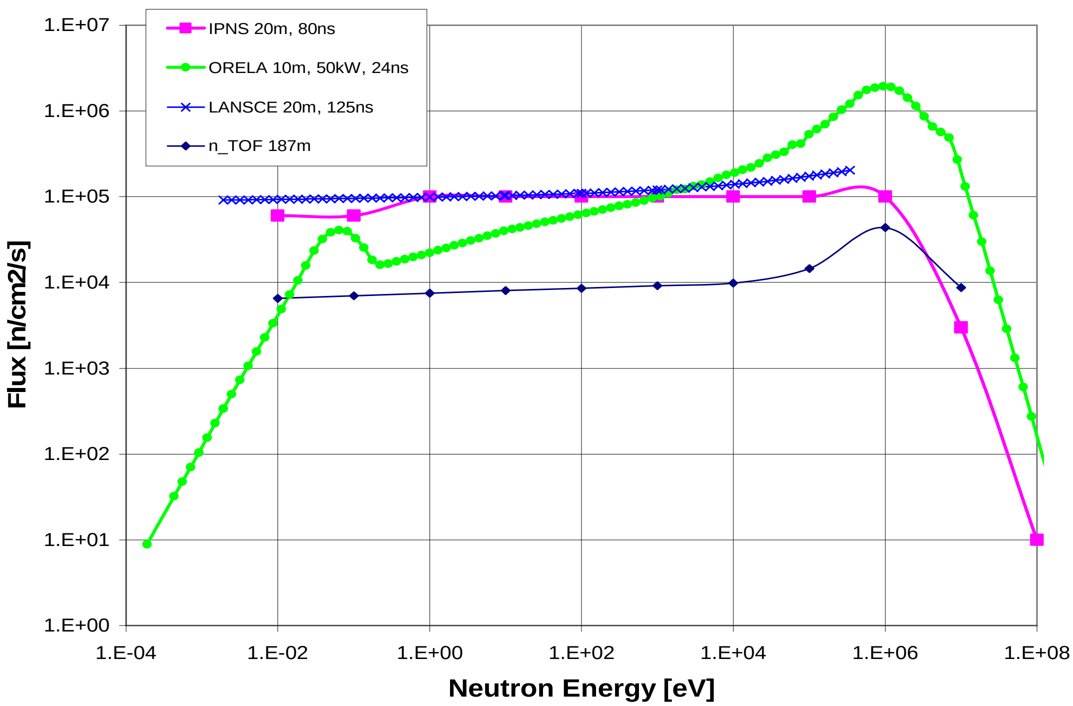

Figure 2. Neutron Flux Spectra of Selected White Neutron Sources.

Table 1: Compilation of the Parameters from Various White Neutron Sources.						
	ORELA	**GELINA**	**RPI**	**LANSCE**	**IPNS**	**n_TOF**
Type of source	electron linac	electron linac	electron linac	spallation	spallation	spallation
Type of particle	e^-	e^-	e^-	p	p	p
Particle energy [MeV]	140	120	>60	800	450	20000
Flight path length [m]	10 - 200	8 - 400	10 - 250	7 - 32	6.2 - 20	185
Minimum Pulse width [ns]	2	1	15	125	70	7
Maximum Pulse width [ns]	30	2000	5000	125	80	7
Maximum Power [kW]	50	11	>10	64	6.3	45
Repetition Rate [Hz]	1-1000	1-900	1 - 500	20	30	0.278-0.42
Best intrinsic Resolution [ns/m]	0.01	0.0025	0.06	3.9	3.5	0.034
Number of Neutron produced [neutron/s]	8.00E+13	3.20E+13	4.00E+13	7.50E+15	8.10E+14	5.35E+14

In mono-energetic sources charged particles are directed at a target of a given material to induce specific reactions that emit neutrons. Several such reactions are ($^{11}B + p \rightarrow {}^{11}C + n$), ($^{7}Li + p \rightarrow {}^{7}Be + n$), ^{239}Pu-Be($\alpha$,n) and ($^{2}H + d \rightarrow {}^{3}He$ n). These reaction spectra are characterized by a narrow high energy peak and a distribution of lower energy neutrons. The energy of the peak can be adjusted slightly by adjusting the energy of the incident particle. A neutron spectrum typical of mono-energetic sources is shown in Figure 3.

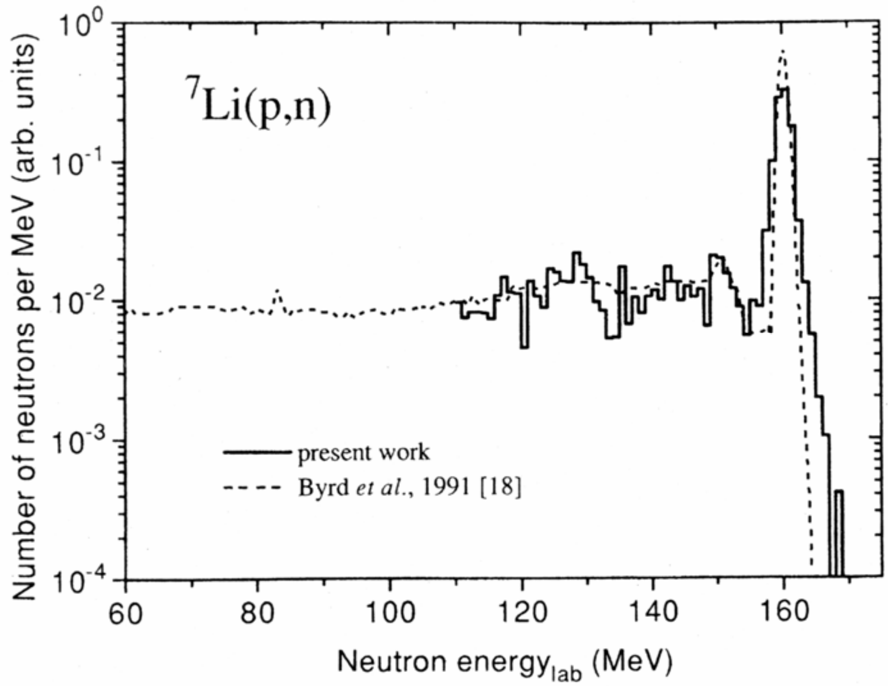

Figure 3. Typical Mono-Energetic Neutron Spectrum. [2]

Neutron Energy Resolution – Time of Flight

In both white and mono-energetic sources the charged particle beams that are bombarded onto the target can be bunched and pulsed. This in turn creates high-flux neutron pulses. These pulses make it possible to calculate the neutron energy by time of flight (TOF) techniques. Pulsing the incident particles makes it possible to determine when they strike the neutron producing target. The neutron-producing reactions are of negligible time scales, and therefore it can be assumed that the instant the charged particles hit the target is the instant when the neutrons are born. Once the time of birth of a neutron is known, its energy can be determined by its spatial location after a certain flight time.

[2] V.P. Eismont, et al., "Relative and Absolute Neutron-Induced Fission Cross Sections of ^{208}Pb, ^{209}Bi, and ^{238}U in the Intermediate Energy Region," Phys. Rev. C 53 (1996) 2911.

For non-relativistic neutrons the particle energy can be found by using

$$K = \frac{1}{2} m_n \left(\frac{L}{t} \right)^2 \qquad\qquad K(eV) = \left(\frac{72.3L(m)}{t(\mu s)} \right)^2$$

where K is the kinetic energy of the neutron,
m_n is the rest mass of the neutron,
L is the length of the flight path of the neutron, and
t is the flight time.

It should be noted that in a vacuum, the flight path is simply the distance traveled by the neutron from the source. Otherwise an additional term has to be included to account for the scattering of the neutrons. This additional term takes into account both the slowing down and the random walk motion of the neutrons. It should be reemphasized that this equation is applicable only for non-relativistic neutrons. If the energies of the neutrons are on the order of a few keV or greater, relativistic corrections need to be used.

The TOF method operates on the assumption that all the neutrons were produced at the same instant. In reality there is a small time period over which the neutrons are produced. This “pulse width” adds uncertainty to the measurement of the neutron energies. For spallation sources this pulse width is typically fixed (between tens of ns and hundreds of ns) and rather wide compared to electron driven neutron sources (pulse width variable between 1 ns and tens of ns), as can be deduced from Table 1. In addition to the pulse width, the moderation time of the neutron and location where it is produced contribute to the uncertainty of the TOF. Spallation neutron sources are usually optimized for thermal neutron flux spectra and are operated with large moderators and a broader pulse. Consequently, the spallation source produces a long tail on the resonances in the resonance region, and these tails are often difficult to correct thereby hindering detailed energy resolution of the resonances. On the other hand, electron driven neutron sources operate with very short pulses and rather small target moderator assemblies. Because electron driven neutron sources also provide long flight paths, they are ideally suited for high resolution cross section measurements in the resonance region. Reducing the pulse width or increasing the flight path of the neutrons will in most cases increase the accuracy of the energy measurement.

After the neutrons are produced they are collimated into a mono-directional beam. This is done by sending the neutrons through a long column that is lined with a strong neutron absorbing material, such as cadmium. This prevents the neutrons that hit the column wall from scattering back into the beam at a different trajectory and energy, and thus contaminating the beam. Mono-directionality is extremely important for double-differential scattering measurements. In these measurements the cross section is measured as a function of both scattering angle and energy. In order to measure the scattering angle the initial trajectory of the neutron needs to be known. The more nearly mono-directional the beam of neutrons is, the better the accuracy of the measurement of the scattering angle will be. Mono-directionality is also important for TOF measurements. If the trajectories of the neutrons vary by a few degrees, the distance the neutrons travel to the target will vary, and the accuracy of the measured energies will decrease.

The neutrons can also be sent through a chopper. This is a device that periodically inserts a strong absorbing material directly into the neutron beam. The neutrons with energies such that they reach the chopper when it is "open" pass through; however, the neutrons that reach the chopper when it is "closed" are absorbed. By adjusting the frequency with which the opening intersects the beam, the chopper can be used as a filter, allowing only neutrons of a particular energy to pass through.

The neutrons are sent through a detector, before striking the sample, to obtain an initial measurement of the neutron flux and spectrum. This flux is used as a control for comparison to the transmitted or scattered beam which is used to determine reaction cross sections. This step can be omitted if the neutron spectrum is nearly constant from one pulse to the next or if measurements relative to some other material are being made. Figure 4 shows a typical apparatus for cross section TOF measurements. The diagram illustrates how various components of the beam line are positioned along the neutron flight path.

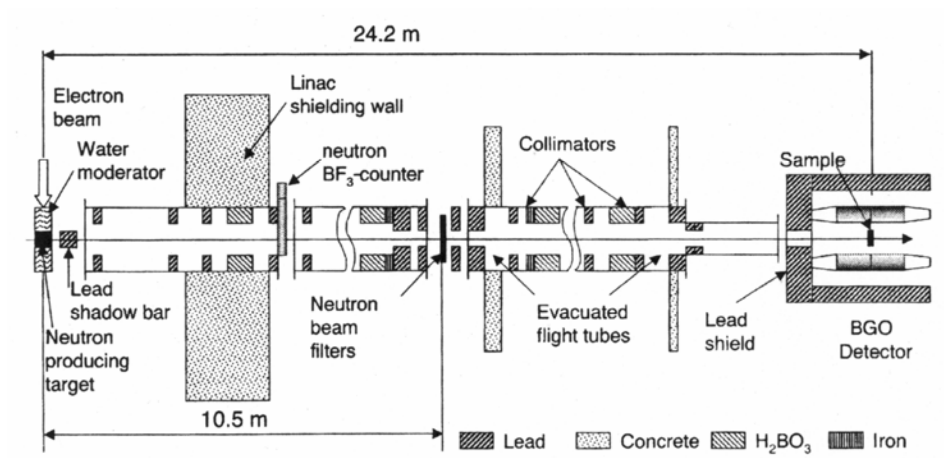

Figure 4. Typical Setup for Neutron Capture Cross Section TOF Measurements. [3]

NEUTRON DETECTION [4]

The detector systems used for cross section measurements can be very complex, but they are all based on one basic concept – allow the neutron to interact with a material that produces a charged particle that then causes ionization in a detector medium. The charged particles are collected to create a measurable voltage or current.

Different materials are used to produce charged particles depending on the energies of the neutrons to be detected. Since the efficiency of a detector depends on the cross section of the chosen material, materials with high cross sections for the production of charged particles are

[3] O. Shcherbakov, et al., "A BGO Detector System for Studies of Neutron Capture by Radioactive Nuclides," Nucl. Instr. And Meth. A 517 (2004) 269.
[4] A more in-depth discussion of radiation detectors consult: Knoll, Glenn F., "Radiation Detection and Measurement," John Wiley & Sons, Inc., New York, 2000.

used. For neutrons at thermal energies, materials such as boron, lithium, and gadolinium are used. Boron is by far the most commonly used material for conversion at thermal energies. ^{10}B has a natural abundance around 20% and boron enriched in ^{10}B is available. The $^{10}B(n,\alpha)$ reaction has a high cross section and releases a high-energy alpha particle (2.792 MeV). The large release of energy also helps to discriminate against background radiation. Many types of boron compounds can be used, including the gas BF_3 which is one of the most common neutron detectors. Detectors using lithium compounds rely on the $^{6}Li(n,\alpha)$ reaction which releases a 4.78-MeV particle. This reaction has a slightly lower cross section than ^{10}B but the higher energy given to the reaction products helps to distinguish events from background.

Fast neutrons can also be measured by reactions that produce charged particles. However, the cross sections of these reactions are typically orders of magnitude less than those for thermal neutrons, resulting in significantly lower detection efficiency. These detectors usually rely on the reactions $^{6}Li(n,\alpha)$ or $^{3}He(n,p)$. Some fast neutron detectors improve their efficiency by using a moderator to slow down the neutrons before they interact with the detector medium. However, the use of a moderator eliminates almost all of the information about the neutrons before they entered the detector and can potentially scatter the neutrons out of the detector before they can be detected.

Another type of fast neutron detector uses neutron induced fission. The advantages of these detectors are that they produce large amounts of energy and that the fission reactions in non-fissile materials, such as ^{238}U, have threshold energies below which fission does not occur. This acts as a natural filter to screen out neutrons that are below the energies of interest.

A third type of fast neutron detector relies on neutron scattering reactions. In elastic scattering the maximum energy that a neutron can transfer to an atom is:

$$E_{\max} = \frac{4A}{(1+A)^2} E_n$$

where E_{max} is the maximum transferable energy,
A is the atomic number of the target nuclei, and
E_n is the initial energy of the neutron.

For recoil detectors lighter elements such as hydrogen and helium are used, because they are capable of receiving a larger fraction of the neutron's energy. The recoil nucleus behaves similar to a proton, and techniques used to detect a proton can be used to detect the recoil nucleus.

Once the neutron has created a charged particle, the neutron detector functions like a standard radiation detector. Radiation detectors can be grouped into three broad categories: multiplication chambers, scintillation detectors, and semiconductor devices.

Multiplication chambers work by applying a large voltage across a gas-filled volume. When radioactive particles strike a gas molecule they have a certain probability of ionizing that molecule. If the gas molecule is ionized both the ejected electron and the ion will be accelerated by the electric field until they collide with and ionize other gas molecules. This cascading process creates a large number of ions that in turn create a measurable current pulse. Each pulse of current corresponds to an electron avalanche. By adjusting the magnitude of the applied voltage the behavior of the avalanche will vary. One type of ionization chamber, the proportional counter, operates in the voltage region where the amplitude of the current pulse is proportional to the energy deposited by the radiation. Geiger-Mueller (GM) detectors, another type of ionization chamber, operate with the voltage set so high that all the gas ionizes and the pulses are all of the same amplitude. In GM detectors all information about the energy of the incident radiation is lost.

Scintillation detectors utilize special materials that emit light when radiation is incident upon them. In these materials, radiation strikes the scintillating medium and excites some of the atoms. The excited electrons then decay to their ground state emitting photons of detectable light, which in turn strike a photocathode which emits electrons (photoelectric effect). The electrons are collected and multiplied by the photomultiplier tube, producing a measurable current. Ideal scintillating materials should emit an amount of light proportional to the energy of the incident radiation, be transparent to the wavelengths of the emitted light, and have prompt decay of electrons back to the ground state. These conditions allow the detector to to be used for both time and energy measurements.

Semiconductor detectors consist of various semiconductor materials such as germanium and silicon that are essentially arranged to form a diode. The ionizing radiation produces free electrons and holes, which are swept out under the influence of a high voltage field to create a measurable current pulse. The energy needed to produce an ion pair in a semiconductor detector is low compared to other detector types, resulting in better statistics and therefore better time and energy resolution. A thorough discussion of semiconductor detectors is beyond the scope of this module, but can be found in many reference texts.

CROSS SECTION MEASUREMENTS

If one looks at *Nuclear Cross Sections* [5] it is obvious that there are many different cross sections that can be measured including (n,γ), (n, tot), (n,2n), (n,f), (n,n') and others. For the criticality safety specialist, the primary cross sections of interest are the fission, capture, scattering and total cross sections.

Total Cross Section

The most basic type of cross section measurement is the transmission measurement of total cross section. This cross section is determined by "simply" measuring the attenuation of a neutron beam by the sample. The intensity of a neutron beam passing through a sample can be expressed by

$$I = I_O e^{(-\Sigma X)}$$

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[5] McLane, Dunford and Rose, *Nuclear Cross Sections, Volume 2, Neutron Cross Section Curves*, Academic Press, Inc., New York, 1988. [The reader may note that this reference has been updated and reissued over several decades and has historically been referred to as "the barn book."]

where I is the beam intensity after passing through the sample,
I_0 is the initial beam intensity,
X is the thickness of the sample,
Σ is the macroscopic cross section of the sample(= $N\sigma$ for a pure substance),
N is the number density of the sample, and
σ is the microscopic cross section of the sample.

Solving the above equation for the macroscopic cross section yields

$$\Sigma = \frac{1}{X}\ln\left(\frac{I_0}{I}\right).$$

A detector is placed behind the sample to measure the neutron beam intensity after passing through the sample. The initial intensity measurement is found by using a flux control measurement as described earlier or simply by measuring without a sample in the beam. When performing transmission measurements, corrections have to be made to account for forward and multiple scattering events as well as various experimental effects. Forward scattering is when a neutron is scattered, but its angle of scattering is not large enough to cause the neutron to miss the detector.

Fission and Capture Cross Sections

Conceptually, the principles of fission and radiative capture cross sections measurements are relatively straightforward; however, fission and capture measurements in practice are technically challenging. Both measurements can be made by surrounding the sample with a 4π detector that detects the radiation emitted in any direction by the capture or fission process. Fission reactions are associated with the release of large amounts of energy (~200 MeV for ^{235}U nuclei from a thermal neutron) making it relatively clear if a fission event occurred and easy to distinguish from background radiation. Those measurements are usually made with an ionization (fission) chamber, which detects the highly energetic fission fragments.

Capture, (n,γ), cross section measurements take advantage of the fact that when a nucleus absorbs a neutron it usually emits one or more gamma rays. These emitted gamma rays have discrete energy levels predicted by quantum mechanical models. By detecting gamma rays at these energies one can determine that capture events have occurred. The emitted gammas are often similar in energy to other common sources of background radiation, and extra care must be taken to shield the system. Work at ORNL has demonstrated that older capture cross section measurement setups exhibited increased neutron background sensitivity due to surrounding structural material (i.e., equipment, detector station housing, etc.). Newer experimental setups have minimal structural material thereby improving capture cross section measurement accuracy.

Scattering Cross Sections

The measurements of elastic and inelastic cross sections are somewhat more complicated since their cross sections are also dependent on the scattering angle of the recoil neutron. To measure these double differential cross sections, $\sigma(E,\theta)$, neutron detectors are placed at various angles around the sample. To maximize the accuracy of the measured angular dependency the neutron detectors are placed as far as practicable from the target. This decreases the number of scattered neutrons that will be detected but higher fluxes are needed to maintain statistical accuracy. The distance between the sample and the detectors is limited by the fact that if the separation distance is too long, then higher energy neutrons scattered in one pulse can catch up and interfere with the lower energetic neutrons scattered in the previous pulse.

Measured Values[6]

Up until now little has been said about what is actually being measured. Historically the measurement of cross sections has been a long process requiring the cooperation of numerous facilities taking months to completely measure one cross section. Considering the energy range (as much as nine orders of magnitude) of most cross sections, and the energy resolution required (especially in the resonance region), it is obvious that the time and money necessary to completely measure the cross sections for even one isotope would be prohibitive. In order to fill in the gaps and to reduce the number of measurements, numerous models have been developed. These models can describe the overall relationship between cross sections and the incident neutron energies, but they contain parameters that need to be experimentally determined. Measurement of cross sections is done to both provide the values of these parameters and to help verify and improve the existing models. In some cases the measurement of an averaged thermal cross section is sufficient. In other cases the measurement of the energies at which resonance peaks occur, their magnitude, and their width is necessary. In more complicated nuclei a measurement of the cross section at a large number of energies is necessary to solve for the parameters and determine the energy-dependent cross sections. Regardless of how well the models are accepted, physical measurements of cross sections are preferred to theoretical data.

Measurement Uncertainties

There are several sources of uncertainty associated with the measurement of any cross section. The most obvious is the presence of impurities or an incomplete separation of isotopes. If a sample is not composed of a single isotope, or if there are impurities present in any significant quantity they will obviously affect the measured cross sections. When multiple isotopes (including impurities) are present the macroscopic cross section has to be found using the relationship:

$$\Sigma = \sum_i N_i \sigma_i$$

where N_i is the number density of the i^{th} isotope, and
σ_i is the microscopic cross section of the i^{th} isotope.

[6] For more information on neutron-nucleus interaction consult Foderaro, Anthony, *The Elements of Neutron Interaction Theory*, The MIT Press, 1971.

Another uncertainty enters when the energy of the incident neutrons is comparable to the vibration states (phonons) of the sample material. These phonons add artificial resonances and are due to the physical properties of the sample, not the nuclear properties. Corrections also have to be made for the possibility that a neutron will scatter off the nucleus of one atom and interact with a second atom. This can be minimized by making the sample as thin as possible. Doppler broadening, another physical phenomenon that has a large effect on measured cross sections, occurs because of the thermal motion of the atoms in the sample. The net effect of Doppler broadening is that as temperature increases the widths of the resonance peaks increase but their maxima decrease. For experiments this can be overcome by cooling the sample to low temperature, e.g. 10 K.

Software packages have been developed by universities and the national laboratories that convert measurement data into usable cross sections including corrections for Doppler broadening, multiple scattering events, background radiation, and isotopic impurities. In order to make the corrections, some basic information on the experimental set up (pulse width, sample composition, flight path, etc.) needs to be included in the input to these codes. The end result of these evaluation codes is an energy-dependent cross section in ENDF format.

EVALUATED NUCLEAR DATA FILES

Once neutron cross section data have been measured, they are evaluated according to a strict set of protocols before being published as an evaluated nuclear data file. Often the evaluation for a given isotope must combine data from multiple researchers and resolve any differences between the measurements. Many times one group will measure high energy cross sections while other groups measure the low energy and resonance regions. Evaluations are performed under the auspices of the Cross Section Evaluation Working Group (CSEWG), which is responsible for production of the U.S. Evaluated Nuclear Data File, ENDF/B. CSEWG is composed of individuals from universities, laboratories, and industry across the U.S. and Canada. Other countries create and maintain their own versions of evaluated neutron data files such as the Japanese Evaluated Nuclear Data Library (JENDL), the Joint Evaluated Fission and Fusion Library (JEFF), the China Evaluated Nuclear Data Library (CENDL), and the Russian Library of Recommended Evaluated Neutron Data (BROND). The ENDF/B format is the standard cross section format used by all of the international nuclear data projects. In addition, researchers in most countries use many of the international cross section sets as a method of comparing evaluations.

The document ENDF-102 (http://www.nndc.bnl.gov/csewg_members/ENDF-102/ENDF-102.pdf) contains a description of all the procedures and formats used in the current ENDF/B files. ENDF/B is organized into various materials and each material contains several files. The first file always contains basic documentation on the cross section and what other files are included for the material. For fissionable materials File 1 also contains the number of neutrons emitted per fission (prompt and delayed) and the energy yields per fission. File 2 contains information on resonance regions. Resonance regions are divided into four groups: Low Energy Region (LER), Resolved Resonance Region (RRR), Unresolved Resonance Region (URR), and High Energy Region (HER). In the LER, resonance and Doppler effects are negligible and the reaction cross sections can be represented as smooth functions. In the RRR experimental techniques are accurate enough to represent each resonance's parameters individually. The resonances in this energy range can be represented by Single-level and Multi-level Breit-Wigner, Reich-Moore, and Adler-Adler approximations. In the URR, experimental techniques are not accurate enough to measure the parameters of individual resonances and averaging functions are used to represent the cross section. In the HER the resonances overlap and the cross section becomes a smooth slowly varying function. Figures 5-8 show the various regions of an ENDF/B plot of ^{235}U fission cross sections.

Notice that the distance between resonance peaks in the RRR decrease at higher energies and then in the URR how the cross section becomes an averaged curve with no discernible resonance peaks.

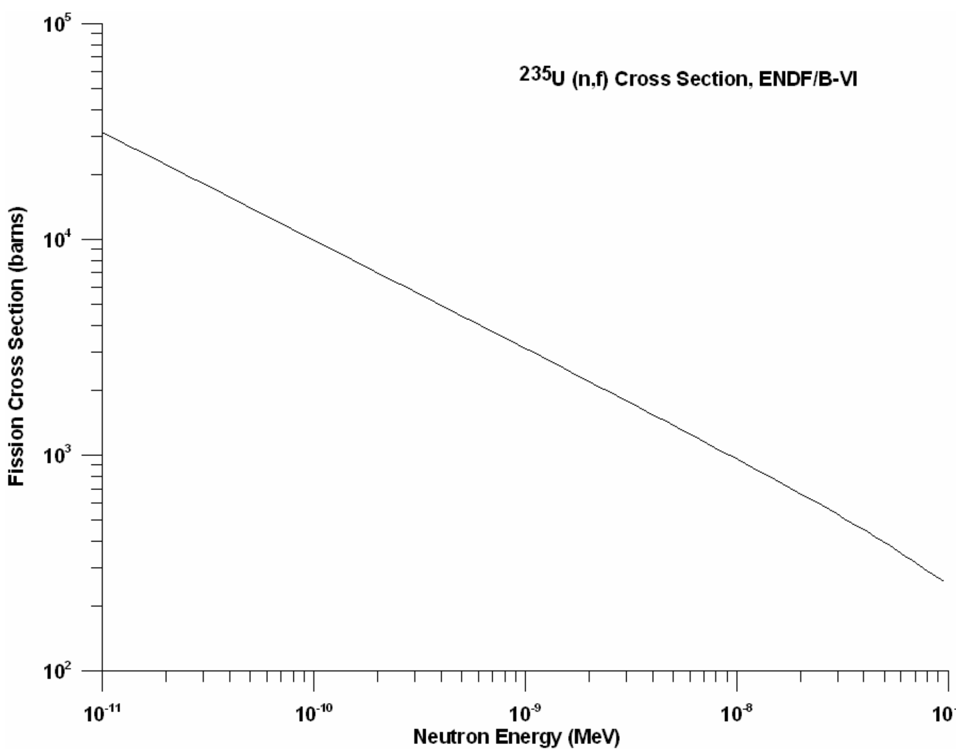

Figure 5. ^{235}U Fission Cross Section in the Low Energy Region.

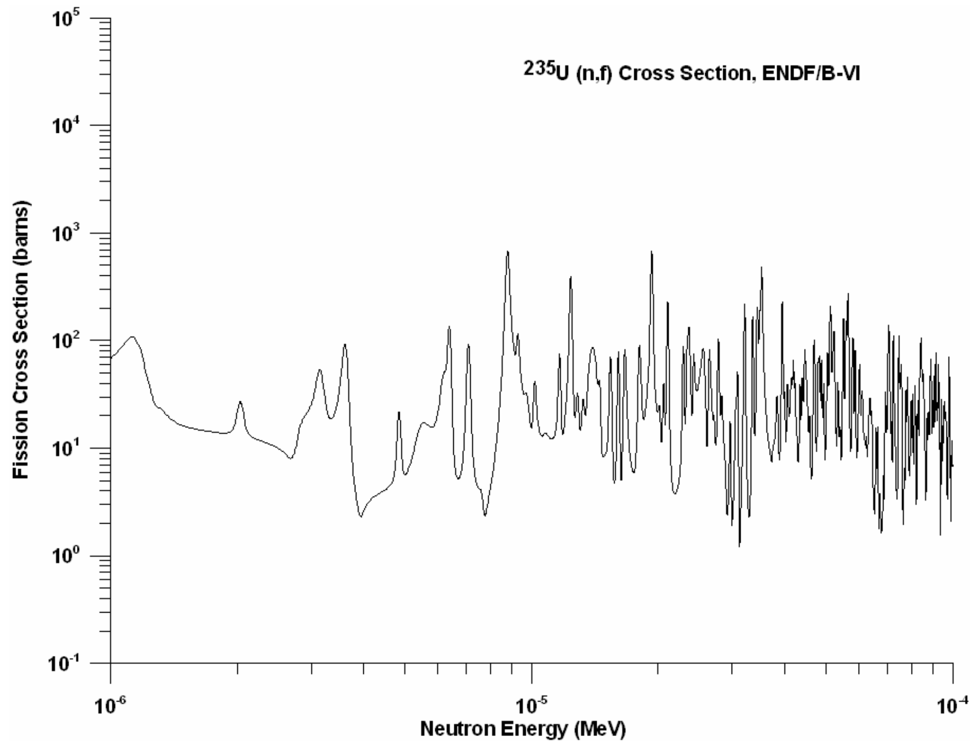

Figure 6. ^{235}U Fission Cross Section in the Resolved Resonance Region.

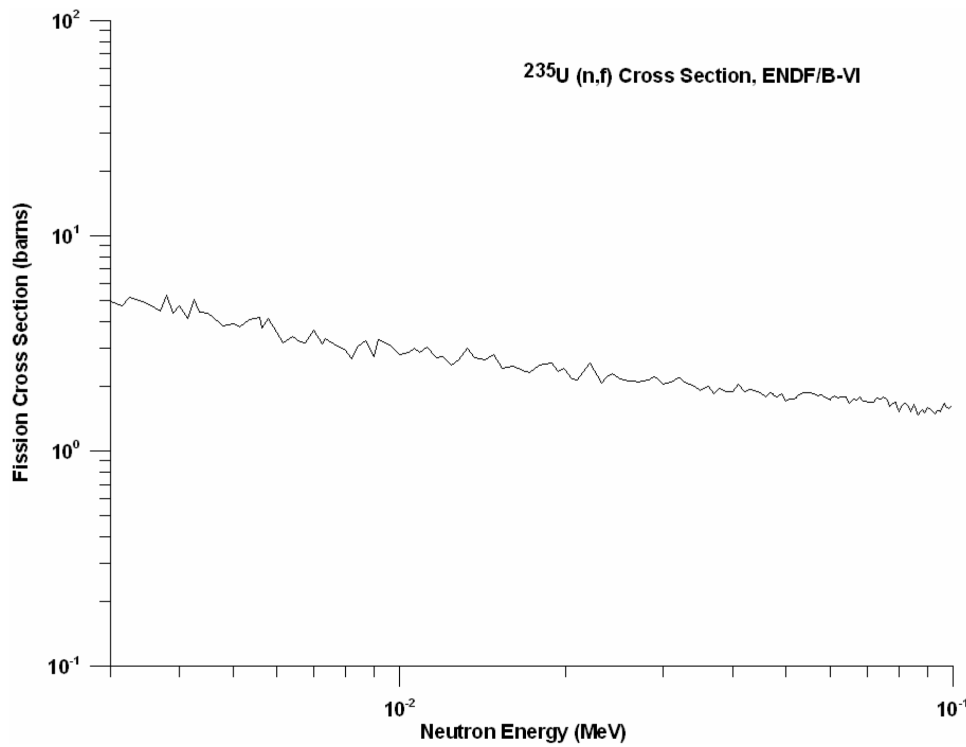

Figure 7. ^{235}U Fission Cross Section in the Unresolved Resonance Region.

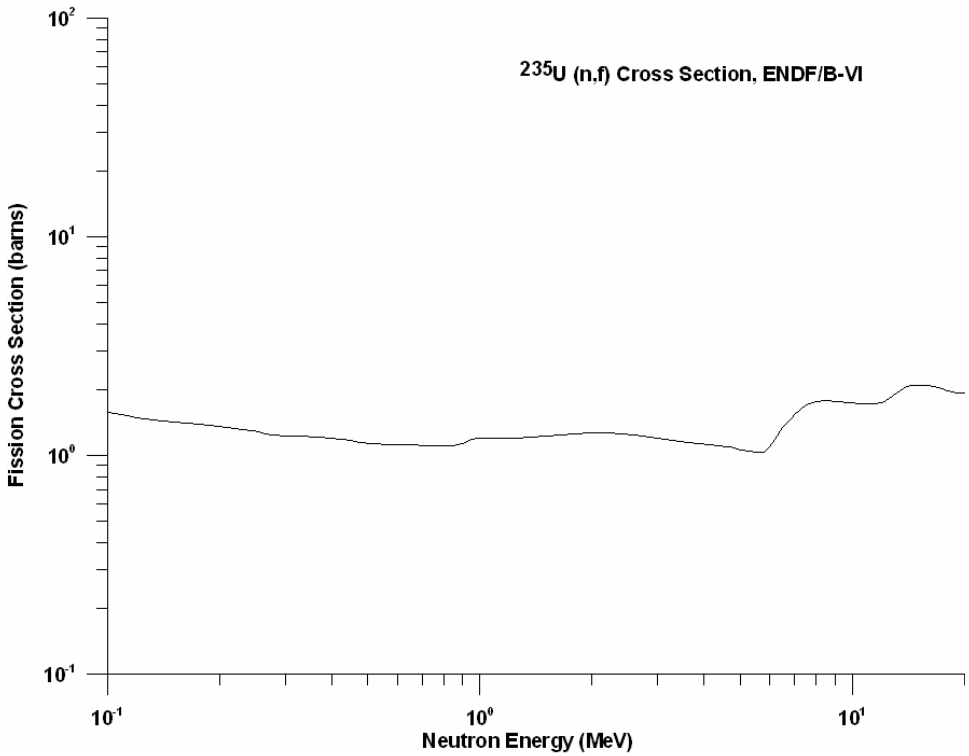

Figure 8. ^{235}U Fission Cross Section in the High Energy Region.

File 3 contains the tabulated cross sections of incident particle reactions. For neutron induced reactions the file must contain cross sections between the energies of 10^{-5} eV to 20 MeV and if possible contain the cross section at .0253 eV. Some reactions have an energy threshold below which they do not occur; for these reactions the cross section does not have to be tabulated below the threshold. The tabulated data are stored in order [E,σ(E)] pairs. ENDF/B uses five different interpolation laws to reconstruct the neutron interaction cross sections between these energy pairs. These laws express σ as constant, σ as proportional to E, σ as proportional to ln(E), ln(σ) as proportional to E, and ln(σ) as proportional to ln(E). Additional ENDF/B files that deal with angular dependence of secondary particles, energy dependence of secondary particles, data covariance, etc. are included when applicable. More information about covariance data is provided in the subsequent discussion. When calculating the actual cross section the resonance data from File 2 must be added to the tabulated date in File 3 unless specifically stated otherwise.

With the advent of modern sensitivity/uncertainty (S/U) analysis software such as the TSUNAMI software in SCALE, the criticality safety analyst has computational tools that can be used to propagate cross section uncertainty or covariance data to a calculated quantity of interest such as k_{eff}. Since the release of Version IV of ENDF, standards and formats have been in place to permit the communication of estimated uncertainties in the evaluated cross section data. The covariance data files provide the estimated uncertainty for the individual data as well as any correlations that may exist. The following list provides a description of the ENDF covariance information and the corresponding file number location within the ENDF system.

File	Covariance Information
31	Average number of neutrons per fission
32	Resonance parameters
33	Neutron cross sections
34	Angular distributions of secondary particles
35	Energy distributions of secondary particles
40	Production of radioactive nuclei

Although significant covariance formats and procedures are in place, the U.S. and international cross section data files have limited cross section uncertainty or covariance data. Previously, S/U tools were not available to use the evaluated covariance data, and cross section evaluators typically did not provide the covariance information due to the substantial effort needed to prepare the data and the perception that the data would not be used. With robust S/U computation tools in place, there is currently a significant demand for cross section covariance data. As a result, there is a concerted effort in the nuclear data community to provide covariance data in cross section evaluations. Currently in the U.S., the covariance evaluation efforts are being led by the criticality safety community, and there is a multi-laboratory effort to prepare covariance evaluations for "high-priority" isotopes/nuclides of interest for criticality safety applications. Note that the cross section evaluation efforts are currently focused on providing covariance information for the average number of neutrons per fission, resonance parameters, and neutron cross sections (i.e., ENDF/B Files 31, 32, and 33, respectively). Currently, S/U analysis tools and cross section processing tools cannot utilize covariance data for secondary energy, angle distributions and the production of radioactive nuclei (i.e., ENDF/B Files 34, 35, and 40, respectively).

As an example, cross section correlation data for the ^{233}U fission cross section in the resonance region is provided in Figure9.[7] The correlation data in Figure 9 are provided in the 44-neutron group structure that is provided with the SCALE code system; however, the energy group boundaries in Figure 9 increase from low to high energies with the increasing group number. Therefore, the lower energy boundary for group 1 corresponds to 1×10^{-5} eV and the upper energy boundary for group 28 corresponds to 100 eV. As shown in Figure 9, the strongest correlations are for cross section energies along and near the diagonal of the matrix. Additional details about ^{233}U covariance analysis are provided in the work by Leal et. al. in Reference 7.

[7] L.C. Leal, G. Arbanas, H. Derrien, N. M. Larson, and B. Rearden, "Covariance Data for ^{233}U in the Resolved Resonance Region for Criticality Safety Applications," *Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications* (M&C 2005) Palais des Papes, Avignon, France, September 12-15, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005).

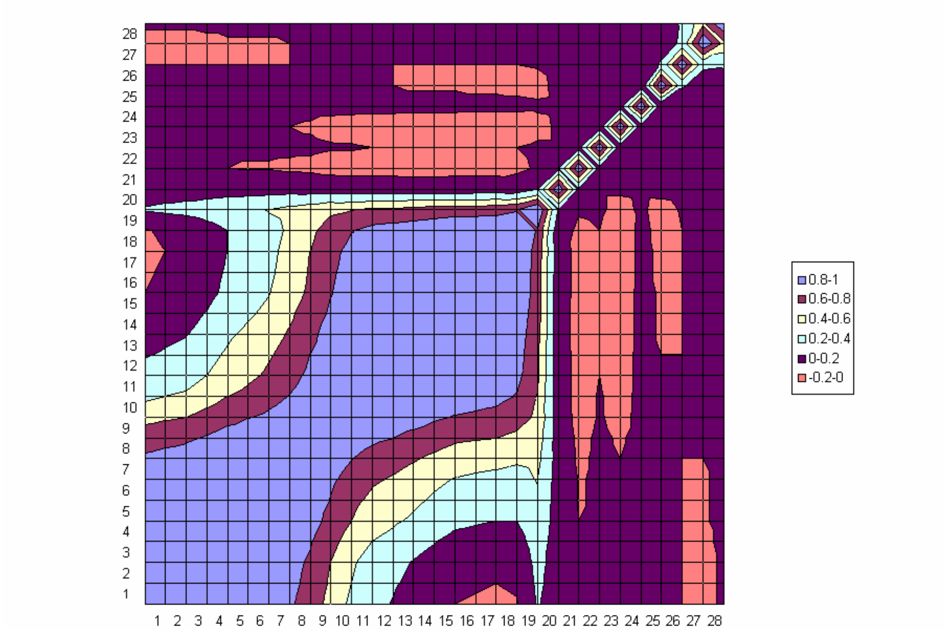

Figure 9. Group Cross Section Correlations for the ^{233}U Fission Cross Section.

There are several steps involved in evaluating a new cross section data file before it is added to the ENDF/B library. First the cross section must be evaluated by considering the available measured data. The evaluated data are generally "fitted" to obtain the best representation of the cross section (or where measurements are not available, the evaluated data are based on nuclear model calculations). The evaluated data are then converted into ENDF/B format. This formatting is generally performed by the same code used to "fit" or evaluate the cross section, such as the SAMMY R-matrix analysis software in the resonance energy range. Then utility codes are used to check the file to make sure it conforms to the ENDF/B format and does not violate any basic physical laws, for instance where the cross section might be negative, where it might be discontinuous, or where energy and momentum are not conserved. After the newly evaluated data file has passed the checking codes, then the performance of the data is tested by comparison to benchmark criticality experiments. If the data file passes all the tests, then it is recommended to be published, i.e., included in the official ENDF/B library. The official ENDF/B data files can be accessed online at the National Nuclear Data Center website, http://www.nndc.bnl.gov/ ; they are also published in Nuclear Data Sheets. The web site also provides convenient tools to display plots of specific reaction cross sections for specified isotopes.

COMPUTATIONAL METHODS AND DATA LIBRARIES

Calculation of an accurate multiplication factor (k_{eff}) for a fissionable system requires that the analysis method provide sufficient rigor in the physics of particle kinematics and cross section data preparation while allowing detailed modeling of the system geometry features.

The particle kinematics of concern in criticality safety calculations involve neutron-nucleus interactions and subsequent secondary neutron energy-angle distributions. These are neutral particle transport processes, and the appropriate physical laws are well understood. A full description of the neutrons in a system can be obtained (in principle) by the solution of the Boltzmann particle transport equation. The solution of this equation can be obtained using statistical (e.g., Monte Carlo) or deterministic (e.g., discrete-ordinates) methods. The kinematics in methods that solve approximations to the Boltzmann equation, such as the diffusion theory model, are not sufficiently rigorous for most criticality safety applications. In any solution scheme it is necessary to have an accurate representation of the energy-dependent cross section structure for each nuclide in a problem. Accurate kinematics modeling requires a combination of good data for the neutron scattering, absorption, and production processes as well as sufficient consideration for the actual particle interaction, including anisotropic scattering. ENDF/B files are general in format and considerable in size. As a result, the ENDF/B files must be processed into smaller data libraries for direct use in radiation transport software. Tools such as AMPX and NJOY are used to process ENDF/B data files and prepare continuous energy (point-wise) and/or multi-group libraries.

In order to reduce the data into usable libraries, cross section processing codes first have to reconstruct the cross sections in the resonance regions using the resonance parameters given in File 2. For the RRR this is done by solving the appropriate representation (Single-level Breit-Wigner, Reich-Moore, etc.) with the given resonance parameters and correcting for Doppler broadening. In the URR the resonance cross section is usually expressed as an averaged function over the region. The resonances are then added to the cross sections from File 3. Then energy points are selected such that when the cross section between the two points is linearly interpolated the discrepancy between the point-wise library and the original ENDF/B file is below some predetermined tolerance. The methods used to determine the grid points vary from code to code, but the points are initially formed by assigning grid points to the maxima, minima, and points of inflections. Then the preparation codes halve the distances between grid points, thus adding additional grid points, until the error is within tolerance. In addition to ENDF/B Files 2 and 3 that describe the energy dependence of the cross section, the processing code must process the collision kinematics data in the ENDF/B file to obtain the exiting energy and angle distributions of secondary particles emerging from a collision. ENDF/B Files 4 and 5 can be used to describe the secondary angle and energy distribution of particles emerging from a collision.

With the release of ENDF/B-VI, a File 6 can be provided to describe coupled energy-angle distributions of particles emerging from a collision. For thermal moderators (e.g., hydrogen in water, graphite, etc.), File 7 is used to provide $S(\alpha,\beta)$ data to describe the thermal scattering process with the moderator material. These collision kinematics files in an ENDF/B evaluation are processed to prepare exit energy and angle distributions for particles emerging from a collision in either continuous-energy or multi-group format. If the ENDF/B evaluation has cross section covariance data, the processing code must process the evaluated covariance data from ENDF/B Files 31, 32, and 33 to prepare covariance data libraries for use in S/U analysis software. Based on the overview of the data library preparation tasks, the cross section processing codes are essential for “bridging the gap” between the basic science data provided in the ENDF/B files and the computational analysis tools that are used to model fissionable systems (refer to Figure 1).

Continuous-Energy and Multi-Group Cross Section Sets

With the rapid increase in computational power of personal computers more analysts prefer programs that use continuous energy libraries such as MCNP, CE-KENO, VIM, etc. In these continuous energy codes, the cross section data and kinematics of the particle interactions are modeled explicitly and the data libraries are preprocessed only to account for temperature effects. Because of the detail in the data libraries, continuous energy libraries are very large due to the number of data points required to represent the structure of the cross section data for each nuclide over the entire energy range. Although continuous energy methods provide rigorous treatment of the underlying nuclear physics, there is a common misconception that continuous-energy transport calculations are free from error. In reality, errors can be introduced into the continuous energy calculation during the preparation of the data libraries. For example, inaccuracies in analyses with continuous energy libraries can result from too few data points or poor processing of the temperature effects. In the case of an overly-coarse cross section energy grid, the detailed structure of the cross section may not be represented correctly (e.g., missing components of the capture cross section resonance, inadequate representation of the “valley” between resonances, etc.). Therefore, the tasks of data preparation, testing and validation are equally important for both continuous energy and multi-group radiation transport methods.

Because of the detailed physics modeling with continuous energy methods, running these codes can still be very time consuming, especially when solving large, complex geometries. As an alternative to using continuous energy methods, the analyst can use multi-group Monte Carlo codes such as the multi-group version of KENO. In reality, all of the deterministic codes and many Monte Carlo codes can solve the Boltzmann transport equation using a multi-group representation. To solve the equation using this multi-group representation requires group-averaged cross sections for each spatial zone. The cross sections are prepared with the criteria that the average reaction rates over each energy group are preserved. Preserving the reaction rates necessitates that a neutron flux spectrum be assumed for the preparation of the group data. Use of a very fine group structure minimizes the impact of the assumed flux spectrum because it is the relative change in the flux across the energy group that affects the "weighting" of the cross section data. Typically the spectrum used to prepare a fine group library (100 groups or more) is a combination of a fission spectrum joined to a 1/E slowing-down spectrum that, in turn, is tied to a thermal Maxwellian spectrum. Fine group libraries can subsequently be collapsed to a broad group structure using a flux spectrum that is consistent with a general class of problems.

The multi-group cross section sets such as those discussed above contain a large amount of information relative to the particle kinematics (e.g., scattering matrices). However, correction of the cross sections for resonance self-shielding (reduced effect of the cross section at an energy point due to the effect of resonances at a higher energy) and Doppler effects (broadening of the cross section resonances due to the thermal motion of the nucleus) is most accurately performed on a problem-specific basis. Resonance processing depends on the amount of material (fissile and non-fissile) in the system, the relative location of the different materials (moderator, reflector, absorbers, etc.), and the condition of the material (temperature, density, etc.). Resonance effects are often extremely important in the calculation of an accurate k_{eff} value; the typical exception is a system where high-energy neutrons above the resonance range dominate. Stand-alone libraries exist that require the user to select the degree of resonance shielding from a set of preprocessed data. This procedure is limited by the user's ability to define the appropriate level of self-shielding for a specific application. The most well-known library of this type is the Hansen-Roach 16-group library that is based primarily on pre-1960s data. Specific processing based on a user description of the system can be provided by data processing code systems such as AMPX and NJOY. Automation of this process as part of a complete problem-dependent analysis is available in the SCALE code system.

Multi-group libraries are created by dividing the energy spectrum into a number of groups and then calculating the average cross section for each group. The number of groups used in a given library will vary depending on the expected spectrum and intended use. In order to find the average cross section for an interval the following expression is used:

$$\overline{\sigma} = \frac{\int \sigma(E)\Phi(E)dE}{\int \Phi(E)dE}$$

where $\overline{\sigma}$ is the group-averaged cross section,
$\sigma(E)$ is the actual cross section at energy E, and
$\Phi(E)$ is the neutron flux at energy E.

In order to solve the above equation the neutron flux as a function of energy is needed. The difficulty comes from the fact that the flux spectrum will differ for each problem and there is no way to know the neutron flux without knowing the cross section. In order to solve for the group-averaged cross section, the historical approach is to assume that the neutron flux will have a particular energy distribution. For example it is commonly assumed that in nuclear reactors the thermal neutrons will have a Maxwellian distribution:

$$\Phi(E) = \frac{2\pi\Phi}{(\pi kT)^{3/2}} E^{1/2} e^{-E/kT}$$

where k is Boltzmann’s constant,
T is the temperature, and
Φ is the total flux over all energies.

When the neutron distribution used to solve for the average flux is close to the neutron distribution of a particular situation, multi-group libraries can give accurate results; but when the two distributions do not match well the results of any calculation will be inaccurate. <u>It is important to select a cross section library that was created for the type of calculation being performed</u>. Libraries designed for thermal reactors should not be used for fast reactor calculations, etc. When selecting a library it is important to select one with the largest number of groups available for that application. By increasing the number of groups, the reliance of the averaged cross section on the averaging distribution is decreased, and the error introduced by the discrepancies between the assumed and the actual neutron distributions is minimized.

More modern multi-group transport software such as the SCALE package has robust problem-dependent solution capabilities that overcome historical difficulties with the multi-group approach. In SCALE, a problem-dependent flux spectrum is calculated in 1-dimensional space prior to solving the Boltzmann transport equation in three dimensions. Specifically, the CENTRM module is used to provide a continuous energy discrete ordinates solution to the transport equation in 1-D for the problem, and the continuous energy flux spectrum is used to prepare group-averaged cross section sets for the problem. As a result, the user is able to prepare problem-dependent multi-group libraries on the fly. Moreover, the CENTRM solution provides a continuous energy cross section treatment for the resonance self-shielding calculation thereby eliminating many of the limitations of historical multi-group transport calculations. As a result, the user gets the benefits of a rigorous continuous energy transport solution to correctly self-shield the resonances and obtain accurate problem-dependent multi-group cross sections. Moreover, the user gets the added benefit of a fast Monte Carlo solution to the transport equation using the multi-group version of KENO.

Deterministic Discrete Ordinates Methods and Monte Carlo Solution Methods

The preceding discussion provides an overview of multi-group and continuous energy data, and the following discussion provides a brief comparison of discrete ordinates and Monte Carlo methods. Computer codes that use the deterministic discrete ordinates technique to solve the Boltzmann equation are very popular for shielding calculations and small-core (high-neutron leakage) reactor physics calculations. The discrete ordinates technique solves for the neutron population on a spatial mesh as a function of discrete energy groups and angular directions. The number of spatial mesh points, energy groups, and discrete angles used to solve for k_{eff} has a direct impact on the computing time and the results. Limiting the groups, quadrature, or mesh to reduce computational time can result in an inaccurate answer for k_{eff}. Angular quadratures, typically referred to as S_n, are based on providing an adequate numerical integration of the angular flux. S_8 and S_{12} quadratures are typical for criticality safety applications. Deterministic codes that solve the integral transport form of the Boltzmann equation can also provide accurate values of k_{eff} for one-dimensional geometries or infinite lattices of uniform cells (spheres, cylinders, etc.). As noted previously, ORNL has developed the continuous-energy discrete ordinates code CENTRM that is used to perform resonance self-shielding calculations to prepare problem-dependent multi-group libraries.

Monte Carlo solution methods involve the use of statistical sampling techniques to "track" neutron histories through scattering and absorption events and then subsequently calculate a k_{eff} value based on the cumulative information from all the histories. Intermediate k_{eff} values are calculated for a batch of neutrons. Early batches of neutrons are typically discarded because they are assumed to be overly biased by the input neutron starting distribution. An estimate of the standard deviation of the k_{eff} value is provided by the code although the k_{eff} value and deviation estimate can be meaningless if the analysis output does not indicate adequate convergence on the predicted k_{eff} value. With the Monte Carlo approach, the neutron kinematics can be treated in either a continuous energy or energy multi-group representation. The burden of ensuring proper particle kinematics shifts in large part from the data processing to the code as one moves from multi-group to continuous energy analyses. Together Monte Carlo methods and discrete ordinates methods provide the analyst with a robust set of computation tools for solving the Boltzmann transport equation for neutron systems.

SUMMARY

Analyses results for a particular model or experiment depend on both the analysis method (i.e., code) and its associated nuclear data libraries. That is, limitations or errors in both the analytical method and in the nuclear data are reflected in biases or errors in the analytical results. This training module has focused on the importance of the nuclear data library and has described the basic processes involved in measuring neutron cross sections, utilizing these measured differential cross sections to produce evaluated nuclear data files, validating or testing the evaluated cross sections for incorporation into the ENDF/B files, and finally processing the ENDF/B data files into processed multi-group or continuous energy cross sections libraries distributed with the various neutronics codes.

Of fundamental importance is the fact that advances (improvements) in cross section measurements, theory, evaluations, processing methods, etc. can only contribute to the improvement of criticality predictions after these improvements have been incorporated into the cross section libraries used by the neutronics codes.