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under Contract DE-AC05-76RL01830

User Guide for the STAYSL PNNL Suite of Software Tools

LR Greenwood
CD Johnson

February 2013

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Richland, Washington 99352

Executive Summary

The STAYSL PNNL software suite provides a set of tools for working with neutron activation rates measured in a nuclear fission reactor, an accelerator-based neutron source, or any neutron field to determine the neutron flux spectrum through a generalized least-squares approach. This process is referred to as neutron spectral adjustment since the preferred approach is to use measured data to adjust neutron spectra provided by neutron physics calculations. The input data consist of the reaction rates based on measured activities, an initial estimate of the neutron flux spectrum, neutron activation cross sections and their associated uncertainties (covariances), and relevant correction factors. The output consists of the adjusted neutron flux spectrum and associated covariance matrix, which is useful for neutron dosimetry and radiation damage calculations.

The software suite consists of the STAYSL PNNL, SHIELD, BCF, and NJpp Fortran codes and the SigPhi Calculator spreadsheet tool. In addition, the development of this software suite and associated data libraries used the third-party NJOY99 Fortran code. The NJOY99 and NJpp codes are used to assemble cross section and covariance input data libraries (for both SHIELD and STAYSL PNNL) from the International Reactor Dosimetry File of 2002 (IRDF-2002) developed by the Nuclear Data Section of the International Atomic Energy Agency (Vienna, Austria). The BCF, SigPhi Calculator, and SHIELD software tools are used to calculate corrected activation rates and neutron self-shielding correction factors, which are inputs to the STAYSL PNNL code.

This report documents each of the software tools, describing the purpose of the software, the installation/uninstallation procedures, the required input data and run options, the type and format of output data, and details of the calculations performed by the software. Because NJOY99 is third-party software, the documentation here of that software is limited to application in the context of the STAYSL PNNL software suite and the user is referred to the NJOY99 documentation for details on general software functionality and implementation.

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1.0 Overview of the Software Suite

The STAYSL PNNL software suite provides a set of tools for working with measured neutron activation rates to obtain neutron spectral adjustment information that can be applied in dosimetry assessments. The software suite consists of the STAYSL PNNL, SHIELD, NJpp, and BCF Fortran codes and the SigPhi Calculator spreadsheet tool developed by the authors at the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. Further, the development of this software suite and associated data libraries uses the third-party NJOY99 Fortran code. While the ancestry of STAYSL PNNL can be traced back to the STAY'SL code by Perey [1, 2, 3, 4], the PNNL version is significantly more user friendly and provides many additional features.

This section provides an overview of the function of each of the software tools and how they are used together for analyzing a set of data. The history of STASYL PNNL and the associated codes is presented to put their development and current status into context. Additionally, a brief overview of relevant concepts is provided to set the stage for discussions of the software. Subsequent sections provide detailed information documenting each of the software tools, including the sources of nuclear data, equations, user input requirements, software operation, and the nature of the resultant output.

1.1 Purpose of and Relationship between the Software Tools

The STAYSL PNNL software suite is comprised of a spreadsheet tool and four Fortran codes, including the namesake STAYSL PNNL. A third-party Fortran code, NJOY99, is used in the process of preparing input data libraries for STAYSL PNNL. Figure 1 shows a simple depiction of the relationship between the software tools, in which the outputs of NJpp, SHIELD, and the SigPhi Calculator are used as inputs to STAYSL PNNL.

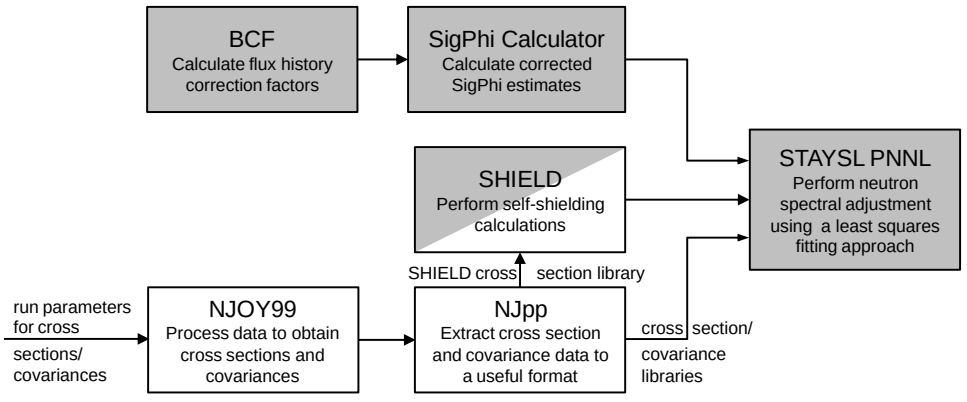


Figure 1. *Sequence of using the software tools in the STAYSL PNNL suite (note that NJOY99 is a third-party software that is used in this sequence of data analysis, but whose code is not included in the suite). Shaded boxes indicate the typical workflow to analyze monitor sample data from a specific irradiation; SHIELD may not be needed if the sample types were analyzed previously for another irradiation.*

In the workflow sequence of Figure 1, NJOY99 and NJpp are key software used to generate cross section and covariance data library files that are used as input to SHIELD and STAYSL PNNL. Because, as discussed below in Section 2.0, the data sources are evaluated nuclear data files and the available reactions are pre-specified, it is anticipated that the cross section and covariance data libraries will be generated infrequently. Cross section and covariance libraries generated by the STAYSL PNNL developers are included in the distribution package for the STAYSL PNNL suite. Thus, it is expected that users will not often need to apply NJOY99 or NJpp. However, these codes are described in this User Guide to allow their application when warranted.

Each application run to analyze sample data from a specific irradiation will typically require the use of the SHIELD and BCF codes and the SigPhi Calculator, as well as STAYSL PNNL. This workflow sequence for data analysis is represented by the shaded boxes in Figure 1. Application of the SHIELD code results in a neutron self-shielding data library that is used as input to STAYSL PNNL. If a neutron self-shielding data library containing data for the reactions and sample device geometry (type, thickness) of interest already exists from a previous SHIELD application run, then SHIELD does not need to be run again to re-generate that data library (hence the partial shading in Figure 1). Although some gamma-ray spectrum analysis software packages can calculate flux history corrections for cases where the reactor power or accelerator beam current is constant over the entire duration of the irradiation, it is recommended that the BCF code be routinely used as a consistent method for determining flux history corrections. The SigPhi Calculator is used to determine activation rate results, corrected for relevant phenomena. These corrected activation rates are used as run input parameters for STAYSL PNNL.

A more detailed depiction of the relationships between data sources (shaded rounded rectangles), initial and intermediate input files, and the software codes (shaded squared rectangles) is given in Figure 2 (on the following page).

The software suite includes tools to assemble input data used by STAYSL PNNL with all correction factors taken into account. The BCF code corrects for the growth and decay of activities during the period of irradiation. The SigPhi Calculator is a spreadsheet-based tool that calculates corrected saturated neutron activation rates from measured activities, accounting for changes in activities with time (from the BCF code), gamma self-shielding, and neutron burn-up. The SHIELD code calculates neutron self-shielding corrections based on device geometry and type of neutron field. Within STASYL PNNL, corrections are applied to the neutron activation cross sections prior to the least-squares spectral adjustment. This approach ensures that the proper corrections are applied without having to iterate on flux-based calculations.

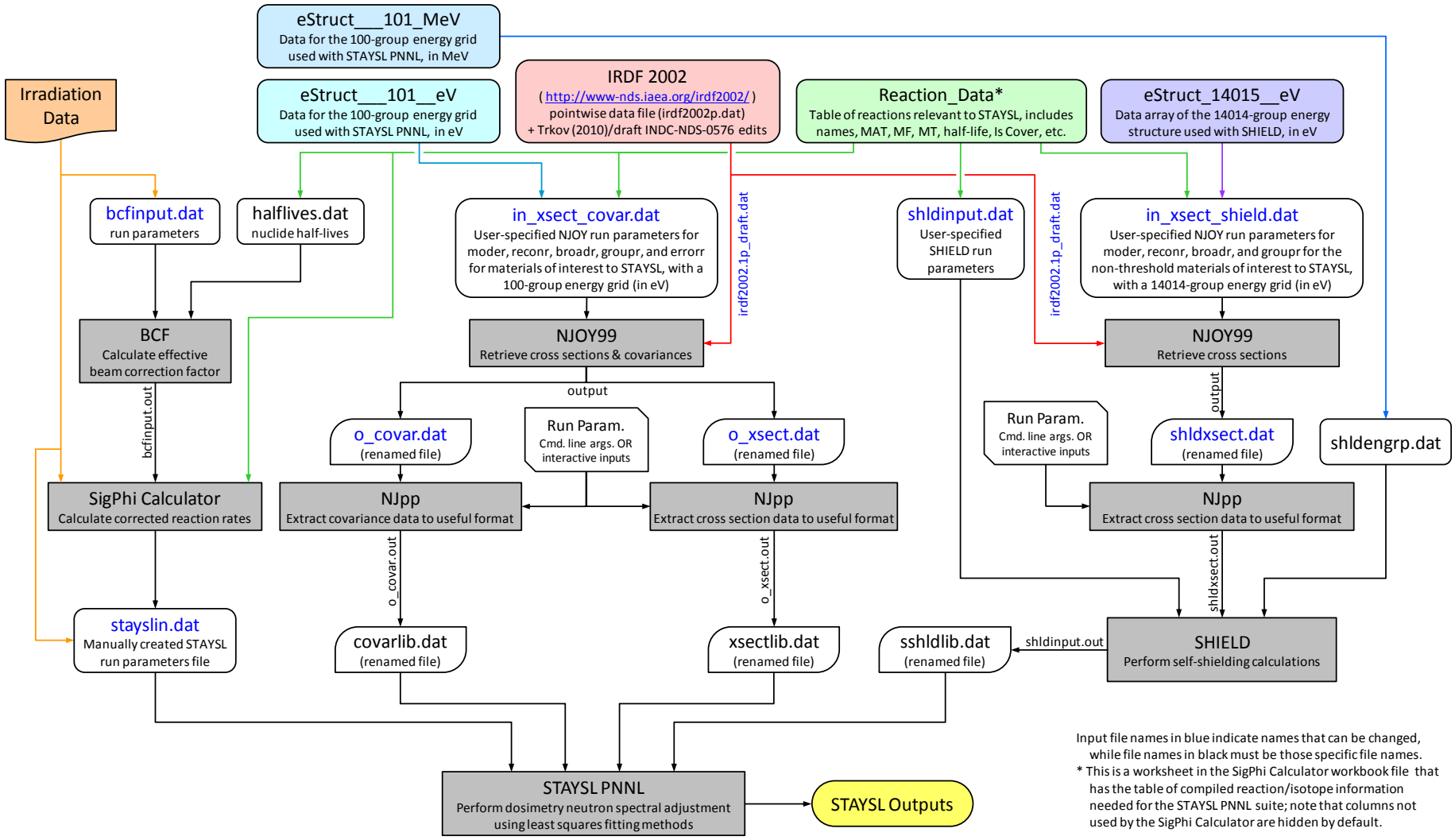


Figure 2. *Detailed relationship between the software tools in the STAYSL PNNL suite, data sources, and input/output files. (Note that NJOY99 is a third-party software that is used in this sequence of data analysis, but whose code is not included in the suite).*

Additional software tools are used to assemble cross section and covariance input data libraries for both the SHIELD code and STAYSL PNNL. The International Atomic Energy Agency (IAEA; Vienna, Austria) Nuclear Data Section's International Reactor Dosimetry File of 2002 (IRDF-2002) [5, 6, 7, 8, 9, 10, 11, 12] provides a standardized evaluated cross section library of neutron dosimetry reactions with uncertainty information. As described in this report, the third-party NJOY99 computer code is used to extract relevant cross section and covariance data from the IRDF-2002 file. The NJpp code is subsequently used to reorganize the extracted information into a format suitable for consumption by SHIELD and STAYSL PNNL. The process of applying NJOY99 and NJpp is not a routine part of the analysis of an irradiation scenario because the cross section and covariance input libraries are not specific to an irradiation scenario and the source library (i.e., IRDF-2002) changes infrequently. The limited circumstances where new cross section and covariance input libraries would be generated using NJOY99 and NJpp include 1) an update/change in the source library, 2) a need to analyze a reaction that is not included in the current SHIELD/STAYSL PNNL data input libraries, or 3) a need to use an energy grid structure other than the defined 100-group grid discussed in this document. Users should recognize that, like any other user-supplied input, the user is responsible for quality control of the supplied data. That is, the quality and reliability of the data libraries generated with NJOY99 and NJpp is dependent on the quality procedures implemented by the user in preparing the root input data.

Given a set of neutron activation rates measured in a nuclear fission reactor or at an accelerator-based neutron source, STAYSL PNNL uses a generalized least-squares approach to determine the neutron flux spectrum. This process is referred to as neutron spectral adjustment [13, 14, 15], since the preferred approach is to use measured data to adjust neutron spectra provided by reactor physics calculations. Application of STAYSL PNNL uses the corrected activation rates calculated in the SigPhi Calculator, the neutron self-shielding correction factors (from SHIELD), the cross section and covariance data libraries (from NJOY99/NJpp), along with the estimate of the neutron flux spectrum (preferably from neutron physics calculations, such those performed by the MCNP[1] code [16, 17]). The output of a STAYSL PNNL application run provides the adjusted neutron spectrum and a brief summary of broader group fluxes and the covariance matrix. Reaction rates and spectral-averaged activation cross sections are also calculated for the convenience of the user for all of the reactions in the nuclear data library. The output can subsequently be used for reactor dosimetry or radiation damage assessments.

1.2 History/Background

Francis Perey developed the STAY'SL code [1, 2, 3, 4] at Oak Ridge National Laboratory (ORNL) in the late 1970s. One of the authors of this current document (Larry Greenwood) had interacted with Dr. Perey over the years to produce a more user-friendly version of the code. One such modification that greatly simplified the input required for each run was to have the code access pre-assembled libraries of nuclear data and the associated uncertainties, instead of requiring the user to specify nuclear data each time the code was run for just the specific

[1] MCNP is a trademark of Los Alamos National Security, LLC, Los Alamos National Laboratory.

reactions being evaluated in the run (as the original version required). Other modifications included improvements to the output files that provide more information to the user, such as broad group and integral flux and fluence values and calculated reaction rates for all reactions in the nuclear data library using the adjusted neutron spectrum. The modernized version of the code is the STAYSL PNNL software described in this document.

Over time, Dr. Greenwood developed the BCF, SHIELD, BURNUP, and BURNS codes to provide important corrections to the reaction rates, which are either applied to STAYSL PNNL input parameter values or within the STAYSL PNNL code calculations. The BCF code corrects activities for decay during irradiation, allowing for very complicated irradiation histories of varying neutron flux and long duration. BCF was originally an acronym for "beam correction factor," but the code developed into a more general tool for both reactors and accelerator beams, while still retaining the BCF acronym. SHIELD corrects for neutron self-shielding for specific monitor sample geometries and neutron flux conditions using nuclear data libraries derived from the same source as for STAYSL PNNL. The BURNUP and BURNS codes correct for nuclear transmutation of the target and product nuclides during irradiation. These latter two (unpublished) codes have been superseded by functionality included in the SigPhi Calculator.

Mr. Johnson (the second author of this report) developed the SigPhi Calculator program as a user-friendly interface for performing corrections to the measured activities and calculating reaction rate (i.e., the so-called "sig-phi") values. The SigPhi Calculator accounts for decay during irradiation (based on BCF), gamma self-shielding, and neutron burn-up (i.e., the functionality of the BURNS and BURNUP codes). The calculated reaction rates of the nuclear reactions of interest for a particular monitor sample are used as input parameters for the STAYSL PNNL code.

The use of NJOY99 and NJpp are more recent developments. NJOY99, a third-party code, has been around for a while, but has only more recently been applied in the process for assembling cross section and covariance data libraries. NJOY 99 extracts nuclear data from evaluated nuclear data files. NJpp, developed by Mr. Johnson, converts the data as extracted by NJOY99 into a compact data library suitable for STAYSL PNNL to access.

As a consultant to the IAEA, Dr. Greenwood produces special-application nuclear data libraries for reactor dosimetry applications. The first library produced was IRDF-90 [18], which was followed by an updated and expanded version called IRDF-2002 [5]. The nuclear data are derived from evaluated nuclear data libraries [19, 20] including ENDF (Evaluated Nuclear Data File), JENDL (Japanese Evaluated Nuclear Data Library), and JEFF (Joint Evaluated Fission and Fusion File). However, the important distinction from general purpose evaluated nuclear data libraries is that IRDF-2002 is a special application file that combines all nuclear reactions that lead to a production of a specific isotope during an irradiation. In the case of inelastic scattering, for example, one must know the sum of reactions to many different excited states that all lead to a longer-lived isomer that can be measured at some time after the irradiation. Similarly, reactions such as (n,np) and (n,d) need to be added together to determine the net production of the activation product that is measured. In the development of IRDF-2002, integral testing data

(such as Cf-252 data) were also considered to ensure the consistency of results in reactor dosimetry applications. Since the publication of IRDF-2002, a new revision of the ENDF library has been published [21] as has the International Reactor Dosimetry and Fusion File (IRDFF) [22]. While the STAYSL PNNL suite doesn't currently use the IRDFF library, future work will likely make use of such resources. Most of the reaction data in IRDFF below 20 MeV are identical to the data in IRDF-2002; the main difference is that IRDFF extends to 60 MeV for applications with higher energy neutron sources.

1.3 Nomenclature and Basic Concepts

This section is intended to give an overview of the nomenclature and concepts relevant to the calculations and function of the software in the STAYSL PNNL software suite, providing a basic framework for conceptualizing the scenarios. Selected works are listed below as a starting point for further reader exploration of neutron reactions, dosimetry, and related topics.

- LANL T-2 website "An Educational Tour of Nuclear Data" [23]
- *Passive Nondestructive Assay of Nuclear Materials* (Chapter 12, "Neutron Interactions with Matter.") [24]
- Journal article entitled "What is neutron metrology and why is it needed?" [25]
- *Handbook of Nuclear Engineering* [26]
- *Handbook of Nuclear Chemistry* [27]
- *Nuclear Energy: Principles, Practices, and Prospects* [28]
- *Neutron Physics* [29]
- *Nuclear Chemical Engineering* (Chapter 2, "Nuclear Reactions") [30]
- *DOE Fundamentals Handbook: Nuclear Physics and Reactor Theory* [31]
- *Industrial Hygiene Engineering* (Section 6.3, "Principles of Ionizing Radiation") [32]
- *Radiation Protection for Particle Accelerator Facilities* (Chapter 5, "Techniques of Radiation Measurement at Particle Accelerators") [15]
- ASTM Standard Procedures [33, 34, 35, 36, 37, 13, 38, 39, 40, 41, 42]
- IAEA Nuclear Data Services documents [43]
- National Nuclear Data Center documents [44]

1.3.1 Basic Definitions

Some definitions are listed below (in groups of related concepts, not alphabetically) to help clarify terms used in this document. Readers are advised to consult standard neutron physics textbooks to gain a more complete understanding of these topics. The ASTM E170 guide [33] is particularly relevant for neutron dosimetry terminology.

radioactive decay – Spontaneous disintegration of a radionuclide accompanied by the emission of ionizing radiation in the form of alpha or beta particles or gamma rays. Given a population of radioactive nuclei at a particular time, N(t), the rate of change in the nuclei due to spontaneous decay is given by the differential equation

shown in Equation 1. Integrating the differential equation gives a first order exponential decay formula (Equation 2).

$$dN = -N(t)\cdot\lambda\cdot dt \quad (1)$$

$$N(t) = N(0)\cdot e^{-\lambda\cdot t} \quad (2)$$

half-life ($t_{½}$) – The time it takes half of an amount of radionuclide to decay; thus, $N(t)/N(0) = ½$ and $t_{½}$ is calculated from Equation 3

$$t_{½} = ln(2) / \lambda \quad (3)$$

decay constant (lambda, λ) – The decay constant for first order decay; calculated from rearranging Equation 3

activity – Radioactive emission rate defined as the number of atoms times the decay constant; dosimeters irradiated in a neutron field are typically (depending on the material/reaction) assayed for activity, which (after corrections) is used as the sig-phi input to STAYSL PNNL

irradiation history – The time dependent production and decay of a given radioactive isotope while in a particular neutron field; the intensity of the neutron flux is nominally linearly proportional to the reactor power (or beam current), so the power (beam current) history is representative of the historical neutron flux conditions

neutron burn-up – Depletion of a given isotope due to nuclear transmutation during irradiation

dosimeter / sample / device – Material used to measure a response when exposed to a neutron fluence; typically in the form of a thin foil or thin-diameter wire

cover material – Material such as boron, cadmium, gadolinium, or gold used to surround dosimeter materials during an irradiation to suppress the thermal and epithermal neutron flux to tailor the response of the dosimeter material to higher energy neutrons

neutron flux (phi, ϕ) – Number of neutrons passing through an area in a given period of time (n/cm^2-s)

neutron fluence (Φ) – Integral of the neutron flux over a specified time period (n/cm^2); integral neutron fluence is when the fluence is also integrated over the entire neutron energy spectrum (i.e., the sum of the neutron fluence for all energy grid groups)

neutron lethargy (u) – Defined as $u = \ln(E_0/E)$, where typically $E_0 = 10$ MeV

reaction rate (sig-phi, $\sigma\phi$) – The saturated reaction rate is the production rate of a given radioactive isotope (product atoms/target atoms-sec). The shorthand notation is sig-phi ($\sigma\phi$) since the rate is equal to the integral over all neutron energies of the group-by-group neutron cross section (sig) times the flux (phi). The measured reaction rate will always be less than the saturated reaction rate due to the growth and decay of radioactive isotopes. Corrections must be made to the measured reaction rate to determine the saturated reaction rate. The reaction rate represents the number of interactions per unit volume and per unit time and can be interpreted as a probability of reaction per unit time.

(non) threshold reaction – A threshold reaction is one that cannot be induced by slow neutrons, where slow neutrons are defined as neutrons below a certain threshold energy. The ENDF-6 manual [45] takes non-threshold reactions as having non-zero cross neutron activation cross section data down to a neutron energy of 1×10^{-11} MeV. For the purposes of the STAYSL PNNL suite of software, a threshold reaction is one with a cross section of 0.0 at a neutron energy of 1×10^{-10} MeV (threshold energies for the reactions used in STAYSL PNNL [see Table 2 in Section 2.3] are all above 0.01 MeV). Otherwise the reaction is non-threshold.

neutron absorption – Removal of neutrons by capture or other nuclear reactions

neutron self-shielding – Bulk neutron absorption in a finite wire or foil such that neutrons are captured on the outer surfaces of the sample and do not penetrate to the center or such that the neutron flux is significantly reduced at the center

neutron spectrum – Distribution of neutron flux (or fluence) versus neutron energy. In a typical light water nuclear reactor, the spectrum can be characterized by a thermal Maxwellian at low energies, a 1/E slowing down spectrum, and a fast fission spectrum at high energies. While the spectrum is a continuous distribution over a range of neutron energies, data is usually tabulated/manipulated for a discretized energy grid

neutron spectral adjustment – Least-squares methodology (contrasted with iterative methods) used by STAYSL PNNL to adjust a calculated neutron spectrum based on measured integral reaction rates

energy grid / groups – Discretization (subdivision) of a neutron energy spectrum into a number of subintervals; the energy grid includes M bins (referred to as groups, the number of which varies depending on the application) and M + 1 energy grid boundaries

thermal neutrons – Neutrons that are in thermal equilibrium with their environment, normally at room temperature of 20 °C = 0.0253 eV; typically follow a Maxwellian distribution (i.e., for thermal motion)

epithermal neutrons – Typically all neutrons having energies between 0.5 eV through 0.1 MeV

fast neutrons – Typically all neutrons above an energy of 0.1 MeV or 1 MeV

2200 m/s – Most probable velocity (v_p) of neutrons in thermal equilibrium at room temperature (20 °C → kT = 0.0253 eV); calculated using Equation 4, where k is Boltzman's constant, m is the mass of a neutron, and T is absolute temperature

$$v_p = \sqrt{\frac{2 \cdot k \cdot T}{m}} = \frac{1m}{100cm} \sqrt{\frac{2 \cdot 1.38 \times 10^{-16} \frac{erg}{K} \cdot 293K}{1.66 \times 10^{-24} g}} = 2200 \, m/s \qquad (4)$$

1/E dependence – Typical shape of neutron energy spectrum in the epithermal energy range, where the neutron flux exhibits an approximate 1/E dependence. That is, if the energy (E) is halved, the flux doubles. The 1/E dependence is caused by the slowing down process, where elastic collisions remove a constant fraction of the neutron energy per collision (on the average), independent of energy.

cross section (sig, σ) – The neutron activation cross section is the probability that a neutron will interact with a target; units are barns (barn = 1×10^{-24} cm^2)

covariance – The relationship between the neutron cross section (or neutron flux) of different energy groups or different reactions

resonance integral – Integral of the neutron activation cross section over a 1/E neutron spectrum from 0.5 eV to 10 MeV

1.3.2 Basic Concepts

The STAYSL PNNL suite of software is used for neutron dosimetry calculations. That is, measurable quantities are assayed from dosimeters that have been placed in a given neutron environment (i.e., a reactor or accelerator beam) and these measurements are used to determine the likely nature of the neutron spectrum to which the dosimeters were exposed. A dosimeter is

a sample (device) in the form of a thin foil or wire of a specific material. When the dosimeter is exposed to neutrons, the neutrons will interact with the dosimeter material and initiate nuclear reactions. The products of these nuclear reactions can be assayed by gamma spectroscopy or other methods. The measured activities can be adjusted to account for factors such as irradiation time or self-shielding. Then, a set of measured activities can be used to adjust an initial estimate of the neutron spectrum to find the most likely neutron spectrum to which the dosimeter samples were exposed.

A key aspect of the dosimetry calculations is the nuclear reaction that occurs between neutrons and atoms of the dosimeter material. Specific reactions are known to occur for specific materials and data about each reaction have been measured, evaluated, and tabulated in nuclear data files. Such nuclear data files are published in standardized forms by agencies in the United States, Europe, and Japan, thereby making data extraction for specific uses relatively straightforward (although some data simply doesn't exist for some reactions). The nuclear reactions that occur can be represented by a general equation. Given a target nuclide (A) and an incoming (incident) particle/quanta (b), the reaction produces an emitted particle/quanta (c) and a product nuclide (D). This generic reaction can be written as $A + b \rightarrow c + D$. Common practice uses the abbreviated notation [29, 46, 47] of A(b,c)D to refer to the reaction, with the parenthetical portion designating the type of reaction. As an example, the (n,p) reaction of a incoming neutron impinging on 26-Fe-54 (i.e., Z-Element-A, where Z is the atomic number and A is the mass number) produces a proton and 25-Mn-54, so this reaction is written as FE54(n,p)MN54.

Figure 3 depicts the types of reactions [24] of interest in neutron dosimetry. Table 1 shows the reaction types (with the above-mentioned parenthetical notation). The table also shows the variant of the reaction type nomenclature used in STAYSL PNNL; the variant is required because STAYSL PNNL can only use ASCII[2] characters. This table also lists the corresponding "MT" numbers that are used to identify the reaction types in ENDF-formatted nuclear data files (see Section 2.2). The specific reactions that STAYSL PNNL can process are described in Section 2.3 (Table 2).

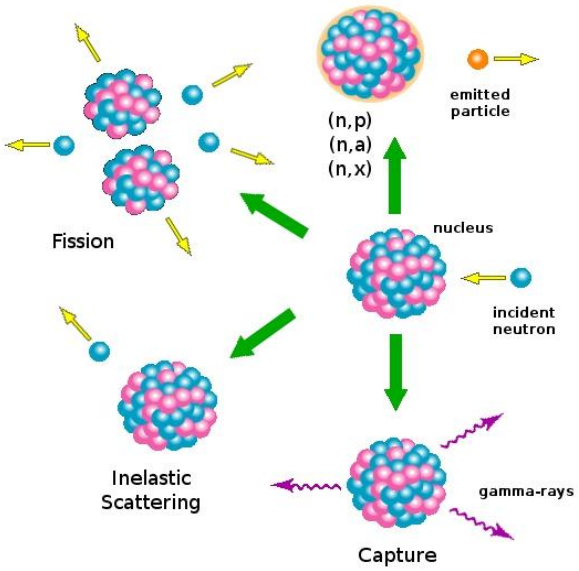


Figure 3. *Depiction of neutron reaction types.*

[2] American Standard Code for Information Interchange (ASCII), as specified in ASA X3.4-1963 [American Standards Association, June 17, 1963] and subsequent standards [e.g., ANSI X3.4-1986, American National Standards Institute, Inc., March 26, 1986].

Table 1. *Description neutron reactions of interest in STAYSL PNNL calculations.*

Type of Neutron Reaction	Reaction Notation [a]	STAYSL PNNL Reaction Nomenclature	ENDF MT Numbers [b]
inelastic scattering	(n,n′)	(N,N')	4 [c]
radiative capture	(n,γ)	(N,G)	102
fission	(n,*f*)	(N,F) or (N,FISSION)	18 [d]
charged particle emission	(n,p) (n,α)	(N,P) (N,A)	105 [e] or 107 [f] 5 [g] or 103 [h]
arbitrary particle emission	(n,x)	(N,X)	5 [g]
sequential decay/three-body breakup	(n,2n)	(N,2N)	16 [i]

[a] Particles are denoted as p (proton), n (neutron), α (alpha particle, helium-4), γ (gamma photon). Fission is denoted with *f*. The notation x is used where one or more particles of any type may be emitted. A numeric value indicates multiple particles of that type (i.e., 2n indicates emission of 2 neutrons).
[b] MT numbers and associated notes are from Appendix B of Herman and Trkov [45].
[c] MT 4 is the sum of MT 50-91.
[d] Particle-induced fission; sum of MT 19, 20, 21 and 38, if present.
[e] Production of a triton, plus a residual; sum of MT 700-749, if present.
[f] Production of an alpha particle, plus a residual; sum of MT 800-849, if present.
[g] Sum of all reactions not given explicitly in another MT number.
[h] Production of a proton, plus a residual; sum of MT 600-649, if present.
[i] Production of two neutrons and a residual; sum of MT 875-891, if present.

Another key aspect of the dosimetry calculations is the neutron flux spectrum to which the dosimeter is exposed. The neutron environment differs depending on the situation (different types of reactors or accelerators), but, generally speaking, the neutrons present encompass a distribution of energies (velocities). The distribution of neutron flux (or fluence) versus neutron energy is the neutron flux (or fluence) spectrum. Characteristic regions of a neutron flux spectrum are a thermal neutron region at low energies, a 1/E slowing down region of epithermal neutrons, and a fast fission region at high energies (Figure 4). The continuous distribution of neutron energies must be discretized (subdivided) into a number of subintervals to make data tabulation and calculations feasible. The discretized energies are referred to as an energy grid that is comprised of M groups (i.e., bins). This converts the integral over the energies to a summation over the energy groups. The number of groups used in the energy grid depends on the particular application; the EPRI-CPM 69-group structure (WIMS structure), VITAMIN-j 175-group structure, and SAND-IIa 640-group structure are some commonly used energy grids [48]. STAYSL PNNL uses a 100-group energy grid (see Appendix B), although SHIELD (Section 5.0) uses a much finer 14014-group structure (to capture the narrow resonance structure in sufficient detail for numerical accuracy). The purpose of STAYSL PNNL is to adjust an initial estimate of the neutron flux spectrum using least-squares methods to find the spectrum that gives the best fit to the measured reaction rates (after corrections).

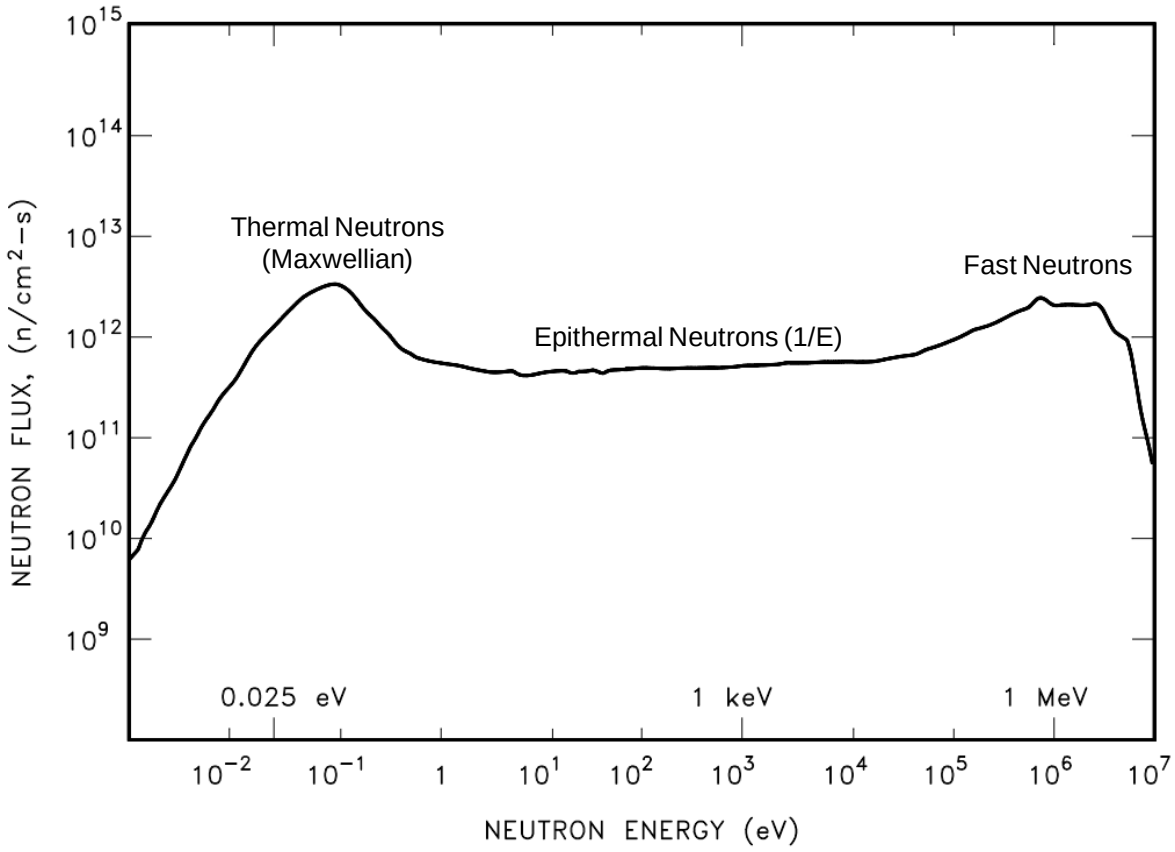


Figure 4. *Example neutron flux spectrum typical of a light water nuclear reactor (after Figure 3 in Module 2 of [31]).*

Each reaction implies not only basic information about the elements involved (i.e., atomic weight, abundance, isotopic composition, half-life, etc.), but also information specific to the reaction. In particular, the probability of an interaction of a neutron with a target, called the reaction cross section, is tabulated for each reaction across the spectrum of possible neutron energies. The neutron activation cross section values are reported in units of barns (where one barn equals 1×10^{-24} cm^2), which are units of area (but which equate to a probability). On an individual target nucleus basis, the probability of interaction is referred to as the microscopic cross section (σ), whereas the cross section for a bulk material (e.g., thin film or wire) is referred to as a macroscopic cross section (Σ). The microscopic and macroscopic cross sections for a given energy level, *i*, are related by the number of target nuclei per unit volume (N) in the dosimeter material, as shown in Equation 5. Figure 5 shows an example of the cross section distribution over a range of incident energies. The least-squares approach used by STAYSL PNNL also makes use of reaction-specific cross section covariance data in determining the adjustment to the neutron flux spectrum. An example of a covariance plot is shown in Figure 6.

$$\Sigma_i = N\cdot\sigma_i \qquad \text{for the } i^{th} \text{ energy level} \qquad (5)$$

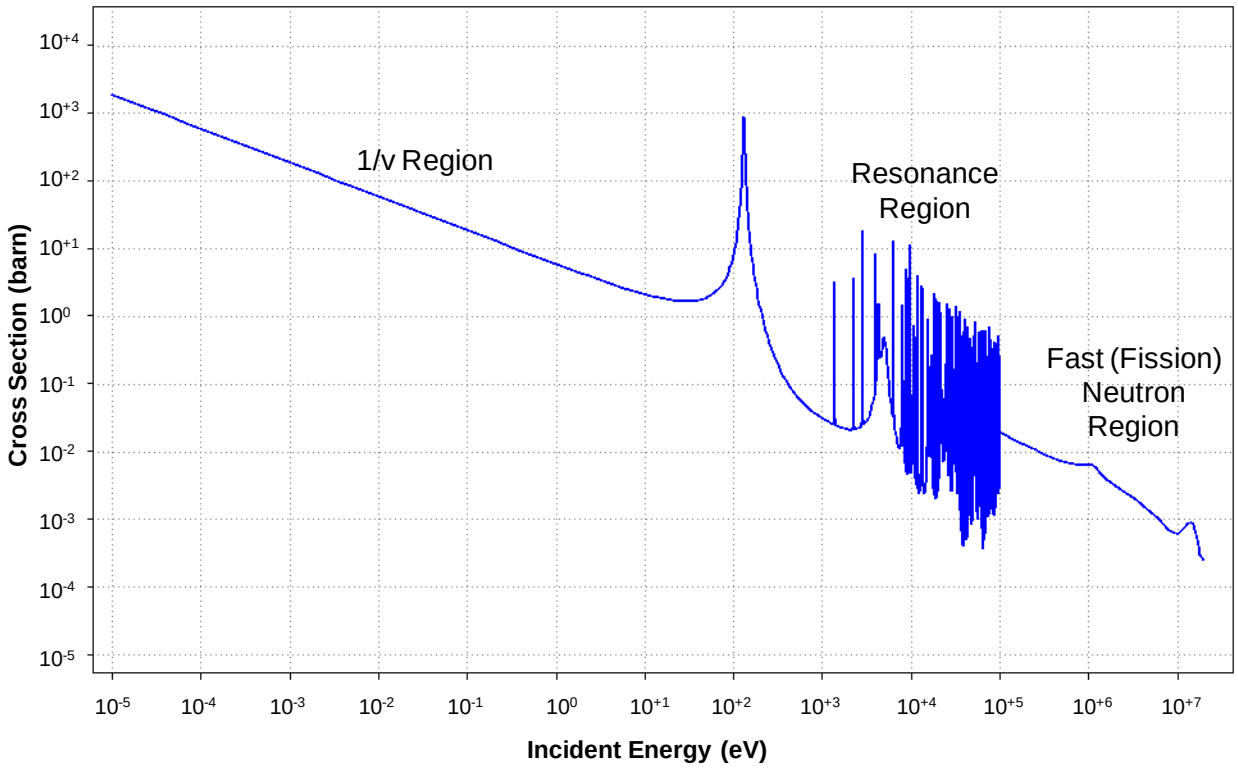


Figure 5. *Plot of the cross section versus energy for the 27-Co-59 (n,g) reaction based on data in ENDF/B-VII.1 (after the plot produced by the NNDC Sigma website utility at www.nndc.bnl.gov/sigma).*

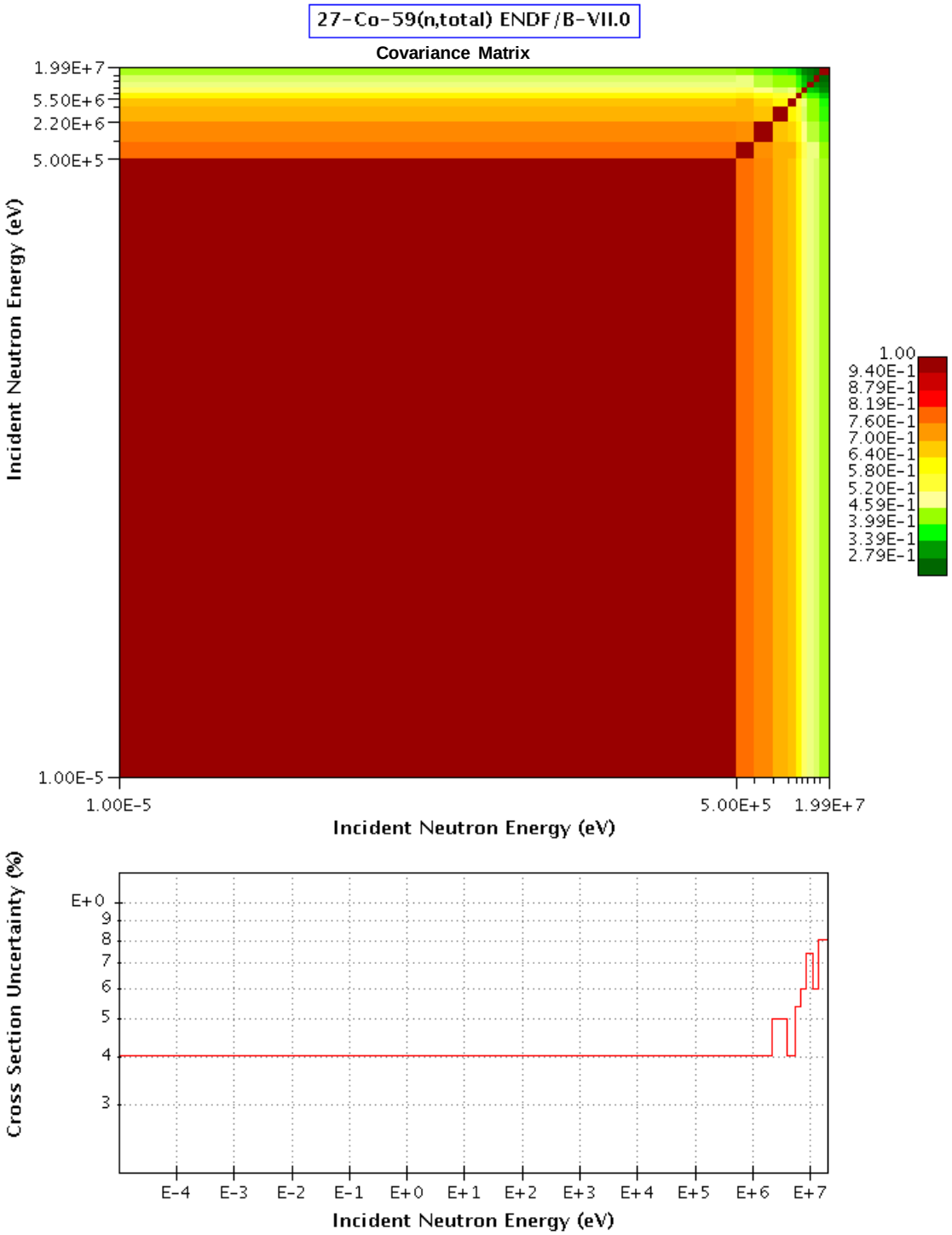


Figure 6. *Plot of cross section covariance and uncertainty for the 27-Co-59 (n,total) reaction based on data in ENDF/B-VII.1 (after the plots produced by the NNDC Sigma website utility at www.nndc.bnl.gov/sigma).*

Reactor dosimetry methods based on integral activation measurements provide a means for determining the neutron fluence in a given neutron environment. Yet, researchers frequently need to determine neutron flux values for a variety of reasons, including comparisons with neutron transport calculations (which always calculate flux values), characterization of a given irradiation facility for planning future experiments, and inter-comparison of different irradiation facilities. The neutron flux is, by definition, determined as the neutron fluence divided by the irradiation time. However, there are multiple conceptual approaches for the nature of the time that is used to calculate the average neutron flux from the fluence (Figure 7). The irradiation time can simply be taken as the actual time from the start to the end of the irradiation, regardless of power fluctuations or downtime (e.g., reactor outages). A less common approach would be to calculate the average neutron flux based on the total operating time (actual irradiation time minus downtime). A third approach (commonly used) is to calculate the effective full power time, which is the irradiation duration that would be required to achieve the same fluence by conducting the irradiation continuously at full power. It is important to remember that the measured neutron fluence is fixed, hence the product of the flux and the irradiation time is invariant, regardless of how the user decides to calculate neutron flux values.

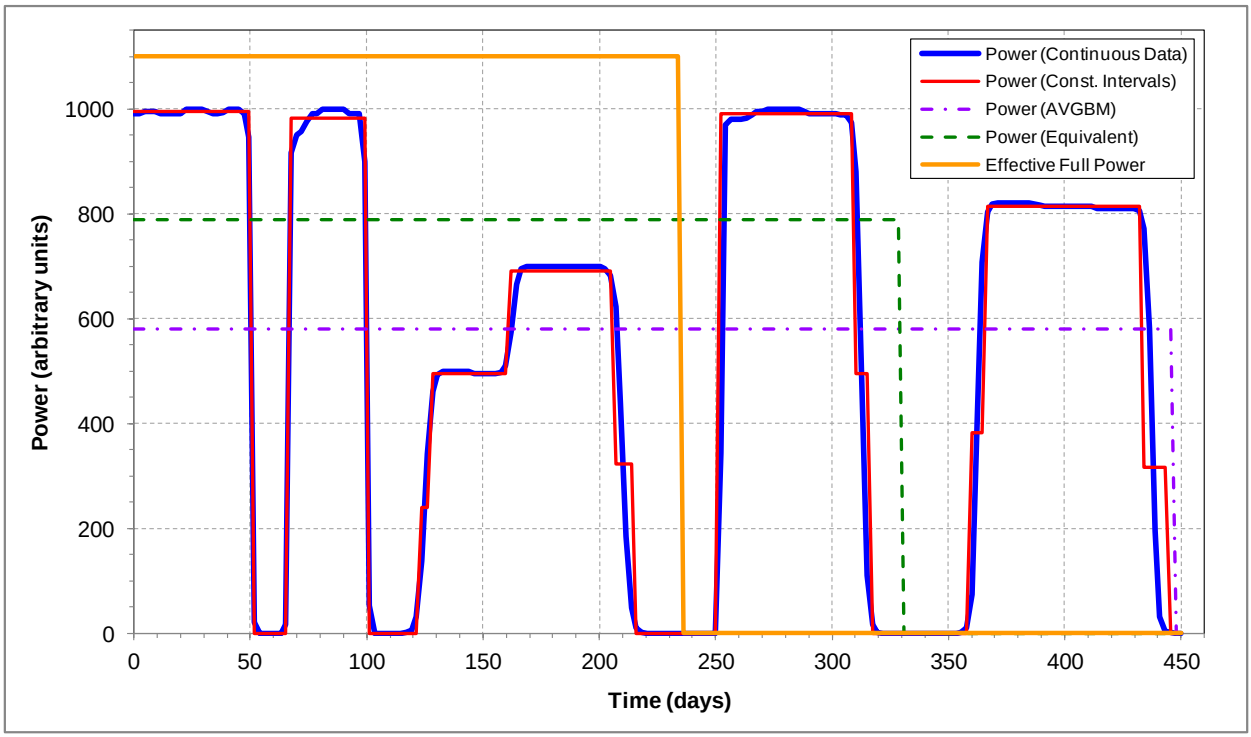


Figure 7. *Example time history of reactor power (arbitrary data/units) with discretization to periods of constant power (Const. Intervals) and several equivalent representations. The variable neutron flux history can be reformulated as the average flux over the total irradiation time (AVGBM), the average flux over the total operating time (Equivalent), or the full power flux over the effective full power time (Effective). While the magnitude of the neutron flux differs, each of these combinations of flux and time result in the same fluence.*

1.3.3 Approach to Applying the STAYSL PNNL Suite

The STAYSL PNNL Software Suite was developed to provide a comprehensive methodology for determining the most likely neutron flux spectrum based on a set of measurements of various neutron activation reactions in any given neutron environment. Measurements are typically performed by exposing high-purity materials to the neutron environment for a fixed period of time followed by gamma counting of the materials after irradiation. The neutron activation data are then converted to activation rates which form a series of integral equations which can be solved to determine the most likely neutron spectrum using a generalized least-squares method. Each measured reaction rate is equal to the integral of the neutron activation cross section times the neutron flux over all possible neutron energies. Since the integral activation rate and neutron activation cross sections are known with specified uncertainties, the only unknown in the integral equations is the neutron flux spectrum. This area of research is more generally referred to as reactor dosimetry and international conferences have been held every 2-3 years on this subject sponsored by the ASTM, EURATOM, and other agencies. The process of determining the most likely neutron spectrum is referred to as neutron spectral adjustment and details are discussed more fully in a variety of references in the literature, most specifically in ASTM standard procedures E262 [35], E720 [36], E844 [37], and related procedures.

The software suite consists of discrete software packages that are designed to give the user all the tools required to perform neutron spectral adjustment. The first step is to create data libraries for neutron activation cross sections and the full cross section covariance matrices. However, data libraries anticipated to be sufficient for most users of this software have been included with the software suite. The nuclear data for these libraries were adopted from the IRDF-2002 [5]. The NJOY99 and NJpp computer codes were used to process the data to create the nuclear cross section library and cross section covariance library files for use by STAYSL PNNL. Information on these programs are included in the package to document the steps used to create the libraries and to provide, for advanced users, a process that could be used to expand or modify the libraries in the future.

For most users of the software, the starting point will be to perform a set of measurements in a given neutron environment. The design of such measurements is discussed in ASTM standard procedures E262 [35] and E844 [37], for example. The measured activities should also be corrected to the end of irradiation time. Once the measurements have been completed, the data need to be converted into what is referred to as saturated reaction rates including a number of correction factors. The term saturated refers to the equilibrium rate that could theoretically be achieved for any reaction given an irradiation time much longer than the decay constant of the product isotope, assuming a constant neutron flux and neglecting neutron burn-up of the target or product nuclides. It is this saturated reaction rate that is equal to the integral of the energy-dependent neutron activation cross section times the neutron flux spectrum. This reaction rate is commonly also called sig-phi, where sig (σ) is short-hand for the neutron cross section and phi (ϕ) is short-hand for the neutron flux. The software and steps for correction of measured activities to sig-phi values for use in STAYSL PNNL are described below.

Activities need to be corrected for decay during irradiation and renormalized to a specified power level (typically to full reactor power, for example). For a very simple irradiation at constant flux, this correction is given by $(1 - \exp(-\lambda t))$, where t is the duration of the irradiation. For more complicated irradiations with varying reactor power and outages, for example, the BCF code follows the ingrowth and decay during each period of constant flux to determine the appropriate irradiation history corrections and normalization factors. The output of BCF is attached to a tab in the Excel spreadsheet.

The SigPhi Calculator is an Excel spreadsheet designed to assist with the calculation of the saturated reaction rates (sig-phi values). The spreadsheet includes all of the corrections that need to be applied to the basic gamma activity measurements. The irradiation history information and renormalization factors from the BCF code are entered into the spreadsheet to account for decay during irradiation. An option to correct for gamma absorption is also included in the SigPhi Calculator. The user needs to specify whether a wire or foil was used for the measurement, but a table of absorption parameters is already included in the spreadsheet. The SigPhi Calculator software also corrects for neutron burn-up of both the target and product nuclide. The basic idea of the burn-up correction method is to use an iterative technique which starts with the measured reaction rate and iterates until the solution converges. Except in the case of very high burn-up corrections, a solution is usually determined within a few iterations. The method further relies on the ratio of reaction rates for the target and product nuclides based on the thermal neutron cross sections and resonance integrals using either a specified ratio of the epithermal to thermal neutron flux or the best fit to this parameter given multiple non-threshold reactions. The SigPhi Calculator spreadsheet also allows the user to correct for neutron self-shielding; however, this is not recommended since this correction can only be determined correctly using an additional program called SHIELD (discussed below).

The output of the SigPhi Calculator is the set of saturated reaction rates, which can be pasted directly into an input file for use with STAYSL PNNL to perform the neutron spectral adjustment. Simple approximations are also used in SigPhi Calculator to give preliminary thermal and fast neutron fluences, but these are rough values for information only.

The SHIELD code corrects for neutron self-shielding for specific monitor sample geometries (foils and wires of particular thicknesses) and neutron flux conditions (isotropic or beam neutron flux) using nuclear data libraries derived from the same source as for STAYSL PNNL. SHIELD uses a fine-resolution 14014-group energy grid to capture the narrow resonance structure in sufficient detail for numerical accuracy in the self-shielding calculations. Application of the SHIELD code results in a data library containing energy-dependent neutron self-shielding factors. This data library is used as input to STAYSL PNNL.

The last step in the process is to run the STAYSL PNNL computer code. The input includes the saturated reaction rates, as determined in the SigPhi Calculator, the output of SHIELD for the neutron self-shielding corrections, and a calculated neutron spectrum. It is highly recommended that the input neutron spectrum be calculated using a neutron transport code such as MCNP using the best information available about the neutron environment being measured. As

mentioned earlier, the proper use of STAYSL PNNL is to then adjust the calculated neutron spectrum based on measured data. Whereas it is often possible to get flux spectrum solutions from STAYSL PNNL that give reasonable agreement to all the data, it must be remembered that such solutions may not be correct if they are not based on basic knowledge of the neutron environment and nuclear physics. Furthermore, the reliability of the adjusted neutron spectrum depends very strongly on the set of measurements that were performed and most reactions have rather broad energy dependence such that it is not possible to determine fine details of a neutron spectrum from a few measurements. The generalized least-squares method, when properly applied, provides the most likely solution to the adjusted neutron spectrum. The output from STAYSL PNNL provides details of the fit to the data, the adjusted neutron spectrum and covariance matrix, integral neutron fluxes and fluences, calculated reaction rates for all of the reactions in the cross section library, files for easy plotting of the data, and files for use with radiation damage computer codes such as SPECTER (see Section 9.0).

1.4 General Software Requirements

The software in the STAYSL PNNL suite falls into two categories: Fortran code and spreadsheet software. STAYSL PNNL, SHIELD, NJpp, and BCF are all Fortran-90 codes, which were compiled and used by the developers using DIGITAL Visual Fortran version 6.0.B3, Compaq® Visual Fortran version 6.6.C, and Intel® Visual Fortran version 10.0 on personal computers of recent manufacture running Microsoft® Windows® XP or Windows® 7 operating systems. NJOY99 is a third party Fortran code developed at Los Alamos National Laboratory (LANL) that was updated using the associated UPD ancillary Fortran code and compiled with the same compilers on the same computing platforms as described above. The SigPhi Calculator is a spreadsheet calculational tool implemented as a Microsoft® Excel® 2003 template file for use in Excel 2003 or Excel 2007. The duration of application runs for of any of the software used as part of the STAYSL PNNL suite are negligible, being at most a few minutes.[3]

Hardware/software requirements to use the STAYSL PNNL software suite are:

Computing Platform:	IBM®-compatible personal computer of recent manufacture
Operating System:	Microsoft Windows XP or Windows 7
Other Software:	Microsoft Excel 2003 or Excel 2007

1.5 General Notes on Installation

The software-specific sections in this document include information on manual installation for each software package. However, the distribution of the STAYSL PNNL software suite will be done as a single "setup" executable file. This installation program will perform multiple installation actions to make the installation seamlessly automated, with the user simply

[3] DIGITAL Visual Fortran was a trademark Digital Equipment Corporation. Compaq was a trademark Compaq Information Technologies Group, L.P. in the United States and/or other countries. Intel is a trademark or registered trademark of Intel Corporation in the U.S. and/or other countries. Microsoft, Windows, and Excel are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries. IBM is a trademark of International Business Machines Corporation, registered in many jurisdictions worldwide.

specifying directories and the software packages of interest. The installation program takes the following actions:

- Places each software package in a subdirectory of the "STAYSL_PNNL_Suite" directory,
- Copies relevant executables to a specified executable directory ("c:\bin\" by default),
- Adds the executable directory to the PATH environment variable,
- Places the SigPhi Calculator Excel template into the appropriate "Templates" directory,
- Configures "Command Prompt Here" functionality when right-clicking on a directory in a file manager (e.g., Windows Explorer),
- Configures "Prepare for STAYSL PNNL" functionality right-clicking on a directory in a file manager (e.g., Windows Explorer),
- Makes a "Start Menu" entry for the User Guide (this document), and
- Makes an uninstall entry for easy removal of all programs.

Thus, while of interest, many of the manual installation actions described for each software package will not need to be explicitly performed. Also, the installation program allows the user to install a subset of the software packages (with NJpp and the PNNL modifications to NJOY99 being two codes that will not typically be needed).

Note that the uninstallation program does not remove the executable directory from the PATH environment variable, nor does it remove the "Command Prompt Here" functionality. The former can be manually performed (e.g., as described in Section 3.2).

The "Prepare for STAYSL PNNL" functionality relies on a batch file installed into the executables directory and simply copies key library files from the appropriate "STAYSL_PNNL_Suite" subdirectories to the indicated directory and concurrently opens a command prompt window at that indicated directory.

At least one "example case" input (and corresponding output) is provided for each software package in the STAYSL PNNL software suite distribution. These files demonstrate the file structures and provide reference files to use for comparison to those produced with the user's installed executables.

2.0 Data Sources

This section describes the sources for tabulated/standard data pertaining to element/isotope properties or nuclear reactions.

2.1 Element/Isotopic Nuclear Data

A variety of tabulated element/isotope nuclear data is used by software in the STAYSL PNNL suite. The BCF code and SigPhi Calculator make use of nuclide half lives from Tuli [49]. The SigPhi Calculator also uses thermal neutron cross sections (σ) and neutron resonance integrals (R.I.) from Holden [50], standard atomic weights of elements from Wieser and Berglund [51], representative isotopic compositions of elements are from Böhlke et al. [52], and relative atomic masses of isotopes are from Audi et al. [53]. SigPhi Calculator and STAYSL PNNL use element densities from Yaws [54]. SigPhi Calculator uses linear mass attenuation coefficients taken from the XCOM database [55]. Fundamental constants, such as Euler's constant and Avogadro's constant, were taken from Cardarelli [56] and Mohr et al. [57], but note that other sources [58, 59, 60, 61, 62, 63] are also of interest.

2.2 International Reactor Dosimetry File 2002

Cross section and covariance data are taken from the IAEA's IRDF-2002 [5, 6, 7, 8, 9, 10, 11, 12] pointwise data library file (available from http://www-nds.iaea.org/irdf2002/). The NJOY99 computer code can be used to extract data from the IRDF-2002 data library because the data is in ENDF format (which is described by Herman and Trkov [45]). Corrections to the IRDF-2002 data library are needed for NJOY99 (Section 3.0) to properly read covariance data for certain materials [11, 12].

Input files for NJOY99 requires some knowledge of the ENDF file format (as well as the NJOY99 input file structure). In particular, the user must know the MAT, MF, and MT numbers for the material/reaction of interest. The convention for assigning MAT numbers is described by Herman and Trkov [45], but is subject to some interpretation and may differ between data libraries. As a guide, MAT numbers for a variety of nuclides (not all in IRDF-2002) were compiled from online data indices prepared by the NJOY99 developers [64, 65, 66] and are listed in Appendix A. Herman and Trkov [45] provide a good description of valid MF numbers (in their Table 0.2) and MT numbers (in their Section 0.5 and Appendix B).

2.3 Data Table

Table 2 lists all of the reactions defined for the STAYSL PNNL suite along with the compilation of data values from the sources described in Sections 2.1 and 2.2. This data table is a static table in the SigPhi Calculator and is used both for the calculations in the SigPhi Calculator as well as for creating the input files for NJOY99.

Table 2. *List of reactions/covers used in STAYSL PNNL with the corresponding nuclear data.*

STAYSL PNNL Short Name	STAYSL PNNL Long Name	ENDF Material ID (MAT)	ENDF File / Info Class (MF) [a]	ENDF Rxn ID (MT)	Threshold Rxn (T) or not (N) and/or Cover (C)?	Target Isotope	Rxn Type	Product Isotope [b]	Target σ (barn/atom)	Target R.I. (barn/atom)	Product σ [c] (barn/atom)	Product R.I. [c] (barn/atom)	Std. Atomic Weight of Target (u)	Rel. Atomic Mass of Target Isotope (u/u)	Isotopic Composition of Target Isotope [d] (mole fraction)	Half-life of Product Isotope [e] (s)
LI6A [a]	LI6(N,A)T [f, g]	325	3	105	N	3-Li-6	(N,A)	2-He-4	940	422	ignore	ignore	6.941	6.0151228	0.0759	--
B	B(N,A)	500	3	107	C	5-B-0	(N,A)	--	--	--	--	--	10.811	--	--	--
B10A	B10(N,A)LI7 [g]	525	3	107	N	5-B-10	(N,A)	2-He-4	3840.315	1730.13	ignore	ignore	10.811	10.012937	0.199	--
F192	F19(N,2N)F18	925	3	16	T	9-F-19	(N,2N)	9-F-18	0.0095	0.021	0.0095	0.021	18.9984032	18.99840322	1.0	6584.76
NA232	NA23(N,2N)NA22	1125	3	16	T	11-Na-23	(N,2N)	11-Na-22	0.43	0.3	28260	200120	22.98976928	22.98976928	1.0	82134965.52
NA23G	NA23(N,G)NA24	1125	3	102	N	11-Na-23	(N,G)	11-Na-24	0.43	0.3	0.43	0.3	22.98976928	22.98976928	1.0	53823.6
MG24P	MG24(N,P)NA24	1225	3	103	T	12-Mg-24	(N,P)	11-Na-24	0.053	0.032	0.053	0.032	24.305	23.9850417	0.7899	53823.6
AL27P	AL27(N,P)MG27	1325	3	103	T	13-Al-27	(N,P)	12-Mg-27	0.23	0.17	0.07	0.03	26.9815386	26.98153863	1.0	567.48
AL27A	AL27(N,A)NA24	1325	3	107	T	13-Al-27	(N,A)	11-Na-24	0.23	0.17	0.23	0.17	26.9815386	26.98153863	1.0	53823.6
P31P	P31(N,P)SI31	1525	3	103	T	15-P-31	(N,P)	14-Si-31	0.17	0.08	0.073	0.033	30.973762	30.97376163	1.0	9438.0
S32P	S32(N,P)P32	1625	3	103	T	16-S-32	(N,P)	15-P-32	0.55	0.25	0.55	0.25	32.065	31.972071	0.9499	1232236.8
SC45G	SC45(N,G)SC46	2126 [h]	3	102	N	21-Sc-45	(N,G)	21-Sc-46	27	12	8	3.6	44.955912	44.9559119	1.0	7239456.0
TI462	TI46(N,2N)TI45	2225	3	16	T	22-Ti-46	(N,2N)	22-Ti-45	0.6	0.4	0.6	0.4	47.867	45.9526316	0.0825	11088.0
TI46P	TI46(N,P)SC46	2225	3	103	T	22-Ti-46	(N,P)	21-Sc-46	0.6	0.4	8	3.6	47.867	45.9526316	0.0825	7239456.0
TI47P	TI47(N,P)SC47	2228	3	103	T	22-Ti-47	(N,P)	21-Sc-47	1.6	1.6	1.6	1.6	47.867	46.9517631	0.0744	289370.88
TI47X	TI47(N,X)SC46	2228	10	5	T	22-Ti-47	(N,X)	21-Sc-46	1.6	1.6	8	3.6	47.867	46.9517631	0.0744	7239456.0
TI48P	TI48(N,P)SC48	2231	3	103	T	22-Ti-48	(N,P)	21-Sc-48	7.9	3.6	7.9	3.6	47.867	47.9479463	0.7372	157212.0
TI48X	TI48(N,X)SC47	2231	10	5	T	22-Ti-48	(N,X)	21-Sc-47	7.9	3.6	7.9	3.6	47.867	47.9479463	0.7372	289370.88
TI49X	TI49(N,X)SC48	2234	10	5	T	22-Ti-49	(N,X)	21-Sc-48	1.9	1.2	1.9	1.2	47.867	48.94787	0.0541	157212.0
V51A	V51(N,A)SC48	2328	3	107	T	23-V-51	(N,A)	21-Sc-48	4.9	2.7	4.9	2.7	50.9415	50.9439595	0.9975	157212.0
CR522	CR52(N,2N)CR51	2431	3	16	T	24-Cr-52	(N,2N)	24-Cr-51	0.8	0.6	10	0.6	51.9961	51.9405075	0.83789	2393496.0
MN55G	MN55(N,G)MN56	2525	3	102	N	25-Mn-55	(N,G)	25-Mn-56	13.3	14	13.3	14	54.938045	54.9380451	1.0	9284.04
FE542	FE54(N,2N)FE53	2625	3	16	T	26-Fe-54	(N,2N)	26-Fe-53	2.3	1.3	2.3	1.3	55.845	53.9396105	0.05845	510.6
FE54P	FE54(N,P)MN54	2625	3	103	T	26-Fe-54	(N,P)	25-Mn-54	2.3	1.3	10	1.3	55.845	53.9396105	0.05845	26967168.0
FE54A	FE54(N,A)CR51	2625	3	107	T	26-Fe-54	(N,A)	24-Cr-51	2.3	1.3	10	1.3	55.845	53.9396105	0.05845	2393496.0
FE56P	FE56(N,P)MN56	2631	3	103	T	26-Fe-56	(N,P)	25-Mn-56	2.8	1.4	2.8	1.4	55.845	55.9349375	0.91754	9284.04
FE58G	FE58(N,G)FE59	2637	3	102	N	26-Fe-58	(N,G)	26-Fe-59	1.3	1.3	13	6	55.845	57.9332756	0.00282	3844368.0
CO592	CO59(N,2N)CO58	2725	3	16	T	27-Co-59	(N,2N)	27-Co-58	37.2	74	1900	7000	58.933195	58.933195	1.0	6122304.0
CO59G	CO59(N,G)CO60	2725	3	102	N	27-Co-59	(N,G)	27-Co-60	37.2	74	2	4.3	58.933195	58.933195	1.0	166344192.0
CO59A	CO59(N,A)MN56	2725	3	107	T	27-Co-59	(N,A)	25-Mn-56	37.2	74	37.2	74	58.933195	58.933195	1.0	928404
NI582	NI58(N,2N)NI57	2825	3	16	T	28-Ni-58	(N,2N)	28-Ni-57	4.6	2.3	4.6	2.3	58.6934	57.9353429	0.680769	128160.0
NI58P	NI58(N,P)CO58	2825	3	103	T	28-Ni-58	(N,P)	27-Co-58	4.6	2.3	1900	7000	58.6934	57.9353429	0.680769	6122304.0
NI60P	NI60(N,P)CO60	2831	3	103	T	28-Ni-60	(N,P)	27-Co-60	2.9	1.5	2	4.3	58.6934	59.9307864	0.262231	166344192.0
CU632	CU63(N,2N)CU62	2925	3	16	T	29-Cu-63	(N,2N)	29-Cu-62	4.5	5	4.5	5	63.546	62.9295975	0.6915	580.2
CU63G	CU63(N,G)CU64	2925	3	102	N	29-Cu-63	(N,G)	29-Cu-64	4.5	5	270	5	63.546	62.9295975	0.6915	45720.0
CU63A	CU63(N,A)CO60	2925	3	107	T	29-Cu-63	(N,A)	27-Co-60	4.5	5	2	4.3	63.546	62.9295975	0.6915	166344192.0
CU652	CU65(N,2N)CU64	2931	3	16	T	29-Cu-65	(N,2N)	29-Cu-64	2.17	2.2	270	2.2	63.546	64.9277895	0.3085	45720.0
ZN64P	ZN64(N,P)CU64	3025	3	103	T	30-Zn-64	(N,P)	29-Cu-64	0.740023	1.4	270	1.4	65.38	63.9291422	0.48268	45720.0
AS752	AS75(N,2N)AS74	3325	3	16	T	33-As-75	(N,2N)	33-As-74	4	61	4	61	74.9216	74.9215965	1.0	1535328.0
Y892	Y89(N,2N)Y88	3925	3	16	T	39-Y-89	(N,2N)	39-Y-88	1.251	1.006	1.251	1.006	88.90585	88.9058483	1.0	9211622.4

Table 2 *continued*

STAYSL PNNL Short Name	STAYSL PNNL Long Name	ENDF Material ID (MAT)	ENDF File / Info Class (MF) [a]	ENDF Rxn ID (MT)	Threshold Rxn (T) or not (N) and/or Cover (C)?	Target Isotope	Rxn Type	Product Isotope [b]	Target σ (barn/atom)	Target R.I. (barn/atom)	Product σ [c] (barn/atom)	Product R.I. [c] (barn/atom)	Std. Atomic Weight of Target (u)	Rel. Atomic Mass of Target Isotope (u/u)	Isotopic Composition of Target Isotope [d] (mole fraction)	Half-life of Product Isotope [e] (s)
ZR902	ZR90(N,2N)ZR89	4025	3	16	T	40-Zr-90	(N,2N)	40-Zr-89	0.014	0.2	0.014	0.2	91.224	89.9047044	0.5145	282276.0
NB93G	NB93(N,G)NB94	4125	3	102	N	41-Nb-93	(N,G)	41-Nb-94	1.1	8.5	15	126	92.90638	92.9063781	1.0	640619280000.0
NB93N	NB93(N,N')NB93M	4125	10	4	T	41-Nb-93	(N,N')	41-Nb-93m	1.1	8.5	1.1	8.5	92.90638	92.9063781	1.0	509024088.0
NB932	NB93(N,2N)NB92M	4125	10	16	T	41-Nb-93	(N,2N)	41-Nb-92m	1.1	8.5	1.1	8.5	92.90638	92.9063781	1.0	876960.0
RH103N	RH103(N,N')RH103M	4525	10	4	T	45-Rh-103	(N,N')	45-Rh-103m	145	1180	145	1180	102.9055	102.905504	1.0	3366.84
AG109G	AG109(N,G)AG110M	4731	10	102	N	47-Ag-109	(N,G)	47-Ag-110m	91.1	1480	82	20	107.8682	108.904752	0.48161	21579264.0
CD	CD(N,G)	4800	3	102	C	48-Cd-0	(N,G)	--	--	--	--	--	112.411	--	--	--
IN115N	IN115(N,N')IN115M	4931	10	4	T	49-In-115	(N,N')	49-In-115m	205	3400	205	3400	114.818	114.903878	0.9571	16149.6
IN1152	IN115(N,2N)IN114M	4931	10	16	T	49-In-115	(N,2N)	49-In-114	205	3400	205	3400	114.818	114.903878	0.9571	71.9
IN115G	IN115(N,G)IN116M	4931	10	102	N	49-In-115	(N,G)	49-In-116m	205	3400	205	3400	114.818	114.903878	0.9571	3257.4
I1272	I127(N,2N)I126	5325	3	16	T	53-I-127	(N,2N)	53-I-126	6.2	150	6.2	150	126.90447	126.904473	1.0	1117152.0
LA139G	LA139(N,G)LA140	5728	3	102	N	57-La-139	(N,G)	57-La-140	9.2	12	2.7	69	138.90547	138.9063533	0.9991	144987.84
PR1412	PR141(N,2N)PR140	5925	3	16	T	59-Pr-141	(N,2N)	59-Pr-140	11.5	14	11.5	14	140.90765	140.9076528	1.0	203.4
GD	GD(N,G)	6400	3	102	C	64-Gd-0	(N,G)	--	--	--	--	--	157.25	--	--	--
TM1692	TM169(N,2N)TM168	6925	3	16	T	69-Tm-169	(N,2N)	69-Tm-168	108	1500	108	1500	168.93421	168.9342133	1.0	8043840.0
TA181G	TA181(N,G)TA182	7328	3	102	N	73-Ta-181	(N,G)	73-Ta-182	20.012001	650.4	8200	900	180.94788	180.9479958	0.99988	9886752.0
W186G	W186(N,G)W187	7443	3	102	N	74-W-186	(N,G)	74-W-187	37	510	70	2760	183.84	185.9543641	0.2843	85392.0
AU1972	AU197(N,2N)AU196	7925	3	16	T	79-Au-197	(N,2N)	79-Au-196	98.7	1550	98.7	1550	196.966569	196.9665687	1.0	532820.16
AU197G	AU197(N,G)AU198	7925	3	102	N, C	79-Au-197	(N,G)	79-Au-198	98.7	1550	26500	40000	196.966569	196.9665687	1.0	232899.84
HG199N	HG199(N,N')HG199M	8034	10	4	T	80-Hg-199	(N,N')	80-Hg-199m	2100	435	2100	435	200.59	198.9682799	0.1687	2560.2
PB204N	PB204(N,N')PB204M	8225	10	4	T	82-Pb-204	(N,N')	82-Pb-204m	0.68	2	0.68	2	207.2	203.9730436	0.014	4104.0
TH232F	TH232(N,FISSION)	9040	3	18	T	90-Th-232	(N,F)	40-Zr-95	7.370004	85	0.19	0.95	232.03806	232.0380553	1.0	5532364.8
TH232G	TH232(N,G)TH233	9040	3	102	N	90-Th-232	(N,G)	90-Th-233	7.370004	85	1515	400	232.03806	232.0380553	1.0	1309.8
U235F	U235(N,FISSION)	9228	3	18	N	92-U-235	(N,F)	40-Zr-95	681.0001	419	0.19	0.95	238.02891	235.0439299	0.007204	5532364.8
U238F	U238(N,FISSION)	9237	3	18	N	92-U-238	(N,F)	40-Zr-95	2.7000044	277.00154	0.19	0.95	238.02891	238.0507882	0.992742	5532364.8
U238G	U238(N,G)U239	9237	3	102	N	92-U-238	(N,G)	92-U-239	2.7000044	277.00154	37	277.00154	238.02891	238.0507882	0.992742	1407.0
NP237F	NP237(N,FISSION)	9346	3	18	N	93-Np-237	(N,F)	40-Zr-95	170.02	654.7	0.19	0.95	237.0	237.0481734	1.0	5532364.8
PU239F	PU239(N,FISSION)	9437	3	18	N	94-Pu-239	(N,F)	40-Zr-95	1022.0003	500	0.19	0.95	244.0	239.0521634	1.0	5532364.8
AM241F	AM241(N,FISSION)	9543	3	18	N	95-Am-241	(N,F)	40-Zr-95	703.15	1514	0.19	0.95	243.0	241.0568291	1.0	5532364.8

[a] MF=3 contains reaction cross sections; the corresponding covariances are in MF=10. MF=33 contains cross sections for radioactive nuclide production and the corresponding covariances are in MF=40.

[b] Shading in this column indicates the following comments for the specified MAT IDs. MAT=325: The reaction product is a combination of 2-He-3 and alpha 2-He-4, but the latter is more common and is thus used here. MAT=525: While the reaction product is 3-Li-7, alpha emissions (2-He-4) are what is actually measured. MAT=9040, 9228, 9237, 9346, 9437, and 9543: 40-Zr-95 is a typical fission product, so its properties are used as an estimate for the half-life and target cross section/resonance integral.

[c] Yellow-shaded entries are not known, so they are assumed to be the same values as for the target. Tan-shaded entries (TH232F, U235F, U238F, NP237F, PU239F, and AM241F reactions) are not known, so they are assumed to be the same values as for natural Zr. Red-shaded entries (CO592 and NI58P reactions) have a 9-hour isomer with a very high burn-up cross section or resonance integral. The blue-shaded entry for the CR522 reaction is a "less than" value.

[d] Shading in this column (for MAT=9346, 9437, and 9543) indicates that the sample for the target isotope is assumed to be isotopically pure (no natural isotopes of this element exist). For impure samples, the user would have to override this value in the calculation inputs (not the data table).

[e] Dashed half-life values for non-cover reactions indicate that the product nuclide is stable, with an infinite half life and a decay constant of zero.

[f] This reaction is also goes by "LI6(N, T)HE4" and "LI6(N, T)A" in the literature, which are also valid names. The short name is typically either LI6A (used here) or LI6T. Note that the IRDF-2002 documentation uses the LI6T and LI6(N, T)HE4 terminology.

[g] The LI6(N,A)T and B10(N,A)LI7 reactions are handled slightly differently in the SigPhi Calculator than other non-threshold reactions. The measured product is 2-He-4, so the assay gives an atoms/g quantity, not a Bq/g activity. For the purposes of calculating the burn-up, these reactions are treated as threshold (fast) reactions and the calculated thermal fluence values are not included in the average thermal fluence used in the burn-up calculation for fast reactions.

[h] Convention would indicate that MAT 2126 corresponds to 21-Sc-45m and 21-Sc-45 would be equated with MAT 2125. However, MAT 2126 was used in the IRDF-2002 library for 21-Sc-45. The user can observe that the data is indeed for 21-Sc-45 based on the ZA and LISO (sometimes referred to as LIS0) parameter values in the data library.

3.0 NJOY99

3.1 Introduction/Background/Purpose

The NJOY99 code is software developed at Los Alamos National Laboratory (LANL) by the T-2 Nuclear Information Service Group (http://t2.lanl.gov/codes/njoy99/). NJOY99 is a Fortran-based code used to extract information from nuclear data library files in the ENDF format. Because NJOY99 is a third-party software, the base code itself is not distributed as part of the STAYSL PNNL suite (although the PNNL modifications to NJOY99 are included). It is important, however, to document the role that NJOY99 plays in the sequence of generating input files for STAYSL PNNL (Figure 1).

NJOY99 can be obtained in code package PSR-480 from the Radiation Safety Information Computational Center (RSICC) [67] or the Organisation for Economic Co-operation and Development's (OECD) Nuclear Energy Agency (NEA) Data Bank [68]. The code package includes NJOY version 99.0 (as both executable file and source code) and the ancillary Fortran program UPD (Portable Update Emulator; version 2.0). The UPD code is used to update the NJOY99 source code using updates provided by the LANL developers (and the PNNL modifications). Once updated, the NJOY99 source code must be compiled using a suitable Fortran compiler.

The following description of the NJOY99 code is taken from the PSR-480 documentation [67] compiled by the Radiation Safety Information Computational Center (RSICC):

> *The NJOY nuclear data processing system is a modular computer code used for converting evaluated nuclear data in the ENDF format into libraries useful for applications calculations. Because the Evaluated Nuclear Data File (ENDF) format is used all around the world (e.g., ENDF/B-VI in the US, JEF-2.2 in Europe, JENDL-3.2 in Japan, BROND-2.2 in Russia), NJOY gives its users access to a wide variety of the most up-to-date nuclear data. NJOY provides comprehensive capabilities for processing evaluated data, and it can serve applications ranging from continuous-energy Monte Carlo (MCNP), through deterministic transport codes (DANT, ANISN, DORT), to reactor lattice codes (WIMS, EPRI). NJOY handles a wide variety of nuclear effects, including resonances, Doppler broadening, heating (KERMA), radiation damage, thermal scattering (even cold moderators), gas production, neutrons and charged particles, photoatomic interactions, self shielding, probability tables, photon production, and high-energy interactions (to 150 MeV). Output can include printed listings, special library files for applications, and Postscript graphics (plus color).*
>
> *NJOY99 consists of a set of modules, each performing a well-defined processing task. Each of these modules is essentially a separate computer program linked together by input and output files and a few common constants. The methods and instructions on how to use them are documented in the LA-12740-M report on NJOY91 and in the "README" file. No new published document is yet available. NJOY99 is a cleaned up version of NJOY 97.107 that features improved consistency between different systems,*

more use of block structures, a consistent set of physical constants and support for the CCC-700/MCNP4C Monte Carlo Program.

There is not a current manual for NJOY99. Rather, the documentation for NJOY99 consists of the NJOY91 manual [69], the "Readme0" file [70], and the "Userinp" file [71] (the latter two are included both with the code distribution package and on the NJOY99 website [72], although the "Userinp" file on the website has been revised to reflect the latest update of NJOY99). The "Readme0" describes the purpose of the program, the distribution files, installation/compilation, machine dependencies, updating the code, and the developer-supplied test problems. The "Userinp" file describes the input specifications for each of the NJOY modules. The NJOY91 manual documents the details of the NJOY modules and generally applies to NJOY99, except where the 'Readme0" or "Userinp" provide updated information. A journal article [48] provides a more recent and extensive discussion on using NJOY for processing ENDF/B-VII data files.

The NJOY99 code, when updated to at least update 364 with the PNNL modifications and then re-compiled, can be used to extract data relevant to the STAYSL PNNL software suite. The PNNL modifications include minor changes to improve software usability. These changes include allowing user-specified input file names (for the NJOY99 run parameters file and the ENDF format library file), changing the errorr module to write more significant digits to the output file (changing from a '6E11.3' format to a '6D12.5' format), eliminating the print-out of elapsed processing time, and changing the output formatting to be more informative/esthetic.

As mentioned in Section 2.2, nuclear cross section and covariance data from the IRDF-2002 data library are used for the STAYSL PNNL suite. The IRDF-2002 data library is in ENDF-6 format and thus consists of multiple data sets and a large amount of annotation, making the library unsuitable for direct use as input to a calculational code. The NJOY99 code can be used to extract just the cross section and covariance data of interest from the IRDF-2002 library into meaningful tables (although those tables still require further processing, as discussed in Section 4.0 on the NJpp code).

3.2 Installing, Uninstalling, Updating, and Starting the Code

NJOY99 is a command line program that does not require any particular installation/un-installation procedures per se on a Windows-based personal computer, although the code must be compiled to include updates. The executable file may be placed in any convenient directory. However, to execute the NJOY99 code, the executable must be found in a directory in the command line window's search path. Generating a NJOY99 executable file requires compiling the Fortran source code with a Fortran compiler designed for the computing platform in use.

The NJOY99 package received from RSICC (or OECD-NEA) should include the following files:

- SRC (NJOY99 source code file with markup for processing by UPD)
- UP0 (update 0 for NJOY99, containing only the program version number)
- UPD.exe (compiled version of the UPD code for updating NJOY99)
- NJOY.exe (compiled version of the NJOY 99.0 code)
- Userinp (text file of NJOY input instructions)

The STAYSL PNNL suite distribution includes a "PNNL_NJOY_Modifications.txt" file that comprises a version number update, machine-specific settings (for Intel Visual Fortran on a Windows platform), and the PNNL modifications to NJOY99 (discussed in Section 3.6).

Installation, including updating the NJOY99 code and compiling to a new executable, involves the following steps. Download the latest update file (e.g., "up364") from the T-2 Nuclear Information Service Group's NJOY99 website [72]. If you use a compiler other than g95, Compaq Visual Fortran or Intel Visual Fortran, then also download a compiler-specific update file. Place downloaded files and the "PNNL_NJOY_Modifications.txt" into the NJOY99 directory (e.g., C:\Apps\NJOY99\). Open the update files (e.g., "up364" and "PNNL_NJOY_ Modifications.txt") in a text editor. Copy the content of the PNNL modifications file to end of the numeric update file (e.g., "up364"), replacing the "*ident vers" section. Modify, if required, the compiler-specific section ("*ident pc_ivf") to reflect settings appropriate for your compiler. Save the modified update file as "UPN" without any file extension. Open a command line window at the NJOY99 directory (or navigate within the command line to that directory). Execute the UPD code by typing "upd" at the command prompt. The UPD program will proceed to incorporate the updates and will produce a set of Fortran *.f files. The Fortran files can then be compiled as is typical for the available Fortran compiler to produce a new "njoy.exe" executable. It is probably useful to name the resulting executable file something like "njoy99.364.pnnl.exe" to indicate that it is (for this example) NJOY99 with update 364 and PNNL modifications.

To use NJOY99 from a command line window, the user must do one of three things: refer explicitly to the executable file with the full path, place the "njoy.exe" file into a directory that is already in the standard search path (e.g., C:\Windows\), or add a specific directory to the search path. To execute NJOY99 with an explicit reference, the user would simply type in the full path and executable name at the command prompt (e.g., "C:\Apps\NJOY99\njoy.exe"). The NJOY99 executable can be copied to a directory already in the search path. To see the available directories, type "path" at the command prompt. A directory can be added to the standard search path through the "System" control panel applet (details vary slightly with Windows versions). In Windows 7, edit the "Advanced system settings", then select to edit the "Environment Variables…". Edit the "Path" variable under the "system variables" section of the window. Add the path to the NJOY99 executable (e.g., "C:\Apps\NJOY99\;") to the front of the semicolon-delimited variable value and click "OK" to exit out of the windows. With the change to the system search path, the user can simply execute the NJOY99 program by typing "njoy.exe" at the command prompt regardless of the currently active directory.

NJOY99 can be uninstalled simply by deleting the associated program files and/or directory (e.g., "C:\Apps\NJOY99\"). If the user altered the standard search path, then the user should manually undo that change.

See also Section 1.5 for information on automated installation of the PNNL modifications file and updates to the PATH environment variable.

3.3 Input Data and Run Options

The documentation discussed above (i.e., the NJOY91 manual [69] and the "Userinp" file) describe the input file specifications for all of the NJOY modules. This section will focus on the input data/run options pertinent to extracting cross section and covariance data to generate appropriate data libraries for STAYSL PNNL.

For the purposes of STAYSL PNNL, the NJOY99 processing is used to extract cross section and covariance data for specific neutron reactions (e.g., the "N,G" reaction of Na-23 to Na-24). STAYSL PNNL requires that cross sections for all reactions of interest be included in a single file (and a second comprehensive file for covariances). Thus, these files represent infrequently changing libraries of data (i.e., include everything in the library and STAYSL PNNL will use whatever information is needed based on the specific run options for a scenario). It is possible to process each material type with a separate NJOY99 input file (providing data for all reactions relevant to that material) and subsequently concatenate the processed output into a single file. However, it is most convenient to assemble a single input file to process all materials (and thus all reactions) into one output file.

NJOY99 requires an input file with run directives/options/data to specify how an ENDF format data library (i.e., IRDF-2002) is to be processed. The input file directives tell NJOY99 which NJOY modules are to be run (and their sequence). Run options vary depending on the module, but generally pertain to information such as material identifier, file unit identifiers, weighting options, tolerances, etc. In addition, it may be necessary to specify certain data, such as the temperature of interest or the energy grid. A single NJOY99 input file can be constructed to specify the moder, reconr, broadr, groupr, and errorr modules. The first module specified is the moder module, which does a one-time conversion of the input ENDF library from "coded" to "blocked binary" format (essentially converting from a Fortran formatted/ASCII text to a Fortran "unformatted" file). The reconr module is specified next to reconstruct pointwise cross sections; all materials can be processed in a single specification of the reconr module. After reconr, each material of interest is processed with the broadr, groupr, and errorr modules, grouped together in that sequence. Typically, the broadr/groupr/errorr modules are specified for materials in the sequence of the MAT identification numbers. The NJOY99 input file ends with a "stop" directive. An example input file for using NJOY99 to obtain both cross section and covariance data from IRDF-2002 is given in Appendix B.

There are two exceptions to the above-described sequence of module instructions in the NJOY99 input file. First, the errorr module is not specified for materials that only represent covers, not reactions (e.g., MAT numbers 500, 4800, and 6400). However, material 7925 is both a cover and has reactions of interest, so the errorr module is specified for this material. Second, the group of broadr/groupr/errorr module instructions for Sc-45 (MAT number 2126) must be placed out of numerical MAT number sequence at the end of the input file to avoid a problem in processing the errorr module. When NJOY99 update 364 processes the errorr module for MAT=2126, a flag is not reset, resulting in a failure of errorr module processing (and program

termination) on the next material. A fix at the line labeled errorj.5883 has been identified by the NJOY developers and will be implemented in a future update to NJOY99.

In the specification of the broadr/groupr/errorr instructions, care must be taken with respect to several items. The temperature specified must be consistent between the broadr and groupr module instructions (300.0 K was used for the processing related to the STAYSL PNNL suite). The same energy grid must be specified for all groupr and errorr module instructions. The correct MF values must be specified for each material (see Table 2) and must be consistent between the groupr and errorr module instructions—that is, a MF value of 3 in groupr corresponds to a MF value of 33 in errorr and a MF value of 10 in groupr corresponds to a MF value of 40 in errorr. Materials 2228, 2231, and 4125 have reactions in both MF 3/33 and MF 10/40, so groupr and errorr module instructions are required for both sets of MF values, but the broadr module instructions are only required once.

There are several differences in specifying an NJOY99 input file to extract data that will be used in the SHIELD code. The energy grid must have a finer resolution when extracting data for SHIELD; an energy grid with 14014 groups was used for this work. SHIELD only uses cross section data (not covariances), so errorr module instructions are not included in the NJOY99 input file (and the issues associated with the errorr module, described earlier, are thus irrelevant). Only materials with non-threshold reactions (Table 2) should be included in the processing, because neutron self-shielding is negligible for threshold reactions. If the MF number for a material is 3, then a specific reaction identifier (MT number) can be specified in the NJOY99 input file (to avoid extracting data for extraneous reactions that are not used in SHIELD). However, if the MF number of interest for a material is 10 (see Table 2), NJOY99 (as of update 364) does not recognize the request for only a specific reaction and will terminate when such a request is made. Thus, the NJOY99 input file must be set to process all reactions for a given MAT number when MF=10 (even if some of the reactions are threshold reactions). Of the materials processed for the STAYSL PNNL suite, MAT=4931 (In-115) is the one case where extraneous threshold reactions are extracted with NJOY99. See Section 4.4 for discussion of how these extraneous threshold reactions are dealt with in the final self-shielding library.

3.4 Running the Code

Running NJOY99 is straightforward. Start the NJOY99 executable from a command line window at the directory of interest as described in Section 3.2. With the PNNL modifications to NJOY99 (Section 3.6), the user is prompted for the ENDF-format data library name and then for the NJOY99 input file name. NJOY99 proceeds with the data processing until successful completion or an error is encountered.

3.5 Output

NJOY99 provides the output requested in a file titled “output” in a format discussed in the code documentation. The output file contains a header with the NJOY99 version number as well as the date/time of the application run. The user will not need to work with this output file other than to rename it appropriately to use as input to the NJpp code (Section 4.0). The data of inter-

est is in the file in tables of group constants at infinite dilution (for cross sections) and relative covariance (for the covariance).

3.6 Calculations/Functionality

In general, the primary function of the NJOY99 code is to extract data from ENDF-formatted files. However, there are certain calculations undertaken in NJOY99, such as the Doppler broadening performed by the broadr module. See the NJOY99 documentation [69, 70, 71] for details of possible calculations undertaken as part of data extraction (in particular for the reconr, broadr, groupr, and errorr modules).

The PNNL modifications include minor changes to NJOY99 that facilitate use of the code. Rather than relying on input from the keyboard or from a file via command line redirection, modifications were made so that NJOY99 prompts the user for input file names. First, the user is asked for the ENDF-format data library name (with "tape20" as the default) and then for the NJOY99 input file name (with "irdf100.dat" as the default). Additional modifications were implemented to improve the formatting of the output from the errorr module, including clean-up of the output table header, an increase in significant digits for covariance values, and adding an additional piece of identifying information to an error message. Because NJOY99 runs in minutes and the time it takes for processing with a particular module is of no importance for the use here, the elapsed run time information printed to the output file is set to a constant value of 0.0. Eliminating variation in elapsed run time in the output file also facilitates comparing two files. The final modification is to change the banner of code information to reflect that the version includes the PNNL modifications.

3.7 Test Cases/Examples

The NJOY99 developers provide a suite of 18 test problems that can be used to verify the functioning of the code. Input and output files for the test problems can be found at the NJOY99 website [72] (note that some files are provided for both Windows and *NIX platforms). The test problems utilize data files included with the NJOY99 distribution (ENI61, EPN14, GAM23, GAM27, T322, T404, T511) as well as additional data files available at the website (dummy252Cf, J33_235U, J33_238U, J33_239Pu). The problems of most interest to the use of NJOY99 in preparing data for the STAYSL PNNL suite are 15-18, although the entire set of test problems is used to confirm proper code functioning.

The batch files provided by the developers to run the test cases will require modification. The file paths (including drive letter) will need to reflect the actual location of the data files. Because of the PNNL modifications to NJOY99 to prompt the user for the input file names, the batch file will also need to use file redirection (via a new intermediary text file) to send the default ENDF library file name ("tape20") and the *.dat (NJOY99 input) file names to the NJOY99 program.

4.0 NJpp

4.1 Introduction/Background/Purpose

NJpp (NJOY post processor) is a Fortran code that parses output from NJOY99 and places cross section or covariance data into a file in a compact structured format that can be read by the SHIELD and STAYSL PNNL codes. The SHIELD and STAYSL PNNL codes make use of cross section and covariance data from the IRDF-2002 library (Section 2.2). NJOY99 is used to extract this data from the ENDF-formatted IRDF-2002 file, as described in Section 3.0. While the output from NJOY99 puts the relevant data into a meaningful tabular format, the information is still not in an annotation-free compacted structure suitable for direct use as input to SHIELD or STAYSL PNNL. NJpp provides the functionality to assemble either a cross section or a covariance library file in the format that SHIELD and STAYSL PNNL expect.

4.2 Installing, Uninstalling, and Updating

NJpp is a command line program that does not require any particular installation/uninstallation procedures per se on a Windows-based personal computer. The NJpp code comes as a compiled executable file "NJpp.exe" that the user can simply place in any convenient directory. However, to execute the NJpp code, the executable must be either located in the active directory from which it is being executed or it must be found in a directory in the command line window's search path. Section 3.2 describes the approaches to starting a command line program and how to modify the system search path (substitute NJpp-specific information for path and executable).

NJpp can be uninstalled simply by deleting the "NJpp.exe" file and/or the associated program directory (e.g., "C:\Apps\NJpp\"). If the user altered the standard search path, then the user should manually undo that change.

NJpp is updated simply by replacing the "NJpp.exe" file with a new file. The NJpp version number and date are displayed when the code is run.

See also Section 1.5 for information on automated installation and updates to the PATH environment variable.

4.3 Input Data, Run Options, and Running the Code

NJpp uses two types of input: the output from an NJOY99 run that contains cross section and/or covariance data, and a set of run options specifying the desired behavior of NJpp. NJOY99 output is described in Section 3.5 and nothing further needs to be done with that file aside from perhaps renaming the file or moving it to a different directory. NJpp run options may be specified either as command line arguments or via interactive prompts. The run option parameters (described in Table 3) differ slightly, depending on whether the user is processing cross sections or covariances. The interactive prompts are provided when the NJpp program is started by simply entering the executable name. Command line arguments (in the same order as

the interactive prompts) are entered as follows (parameter names are in angled brackets, parameters entered depending on the processing mode are in square brackets):

NJpp.exe <Fname> <bCovMode> <M> <N> <P> <bMeV> <sFmt> [<bCross>] [<vCover>]

Table 3. *Description of NJpp run option parameters, including default values.*

Input Parameter	Description & Constraints	Default Value
Fname	Name of the NJOY99 output file to process	—
bCovMode	Logical flag specifying whether to process covariances (True) or cross sections (False)	True
M	Energy grid size (number of energy groups, not boundaries) If M is too large (relative to the data in the NJOY99 output file), then NJpp continues with the smaller energy grid specified in the NJOY99 output. If M is too small for the NJOY99 output, then NJpp terminates. For covariance processing, the maximum value of M is 699.	100
N	Maximum number of reactions per material in the NJOY99 output Based on Table 2, N = 3. However, moderate overestimation is fine, and the default value should be used. Underestimation results in an error.	10
P	Maximum number of materials with data in the NJOY99 output Based on Table 2, P = 50 for STAYSL PNNL libraries, and P = 21 for the cross section library used with SHIELD. However, moderate overestimation is fine, and the default value should be used. Underestimation results in an error.	70
bMeV	Logical flag specifying whether to divide the energies by 1E6 (True) or not (False), thereby converting from eV to MeV For the STAYSL PNNL and SHIELD libraries, this parameter will always be True.	True
sFmt	Fortran format specification (as a text value) for a REAL number This format specification is applied to NJpp output in a 7-number wide, wrapped array (cross sections) or a M+1 wide data matrix (covariances)	ES12.5
bCross	Logical flag specifying whether (True) or not (False) to print cross-reaction covariance matrices This parameter is only required when processing covariances. For the purposes of STAYSL PNNL and SHIELD, this parameter must always remain False.	False
vCover	Identifier specifying which covers to process This parameter is only required when processing cross sections. Relevant covers (limited to Au, Gd, Cd, and B; MAT numbers 7925, 6400, 4800, and 500, respectively) can be specified in one of two ways. One approach is to provide an integer value calculated as the sum of the following values for active covers: Au=8, Gd=4, Cd=2, B=1. The second approach is to provide a 4-character string using characters '0' for off and '1' for on, in the order of Au Gd Cd B (left to right).	1111 (equivalent to a value of 15)

4.4 Output

NJpp produces two output files: a diagnostic file and a data library. The diagnostic file contains a list of the reactions that were processed by NJpp and is really just an ancillary product potentially useful for reference. The data library file is the primary output from NJpp and is used as input to the SHIELD code or the STAYSL PNNL code. The structure of the output file is different, depending on whether cross section or covariance data is being processed. Figure 8 describes the output file structure for cross section mode output and Figure 9 describes the output file structure for covariance mode output.

As mentioned in Section 3.3, there are NJOY99 limitations (as of update 364) in processing the input data for extracting cross sections for SHIELD. This results in extraneous threshold

reactions for In-115 (MAT=4931) in the NJOY99 cross section output, and hence in the NJpp output. To avoid inadvertent misuse of the self-shielding library, the "IN115(N,N')IN115M" and "IN115(N,2N)IN114M" reaction cross section data is manually removed from the library produced by NJpp.

Record 1: <Number of energy structure boundaries, M+1> <format specification, sFmt>
Record 2: <Array of energy structure boundary values, 7 columns wide, using specified format, wrapping to next line>
Record 3: <Number of covers>
Record 4: <Cover short name>
Record 5: <Array of cover cross section values, 7 columns wide, using specified format, wrapping to next line>
— Repeat records 4 & 5 for each cover —
Record 6: <Number of reactions>
Record 7: <Reaction short name> <Reaction long name>
Record 8: <Array of reaction cross section values, 7 columns wide, using specified format, wrapping to next line>
— Repeat records 7 and 8 for each reaction —

Figure 8. *Structure of the NJpp output file from an application run in cross section mode.*

Record 1: <Number of energy groups, M> <format specification, sFmt>
Record 2: <Array of energy structure boundary values, using specified format, all values on one line>
Record 3: <Number of materials> <Total number of covariance matrices> <Max. number of reactions per material>
Record 4: <Number of covariance matrices for current material>
Record 5: <Reaction long name>
Record 6: <Array of covariance values, using specified format, with each row of matrix on one line, M lines total>
— Repeat records 5 & 6 for each covariance matrix of the current material —
— Repeat the group of records 4-6 for each material —

Figure 9. *Structure of the NJpp output file from an application run in covariance mode with bCross = False.*

4.5 Calculations/Functionality

NJpp is a data processing code that is used to convert data in NJOY99 output file format to a compacted format structure suitable for use with SHIELD and STAYSL PNNL. The primary functions of NJpp are to parse the NJOY99 output file to find the requested data (cross sections or covariance), convert the energy grid in the NJOY99 output file from eV to MeV (if desired), convert the MAT/MT identifiers into defined reaction names used by STAYSL PNNL, and produce a library data file in a format that SHIELD and STAYSL PNNL recognize.

The only calculation performed by NJpp is to convert the energy grid values from eV to MeV by dividing each value by 1×10^{6}.

The NJOY99 output file is parsed by looking for key phrases, then interpreting the NJOY99 output file structure to extract the relevant data. The energy grid is found by looking for the first instance of the phrase "neutron group structure.....read in", which immediately precedes a table of the energy grid structure. Reactions associated with a material (identified by MAT number) are processed in the same order in which they are found in the NJOY99 output file (note the

discussion of MAT=2126 in Section 3.3). Each instance of "processing mat" identifies the MAT number of the subsequent data tables. The MAT number, along with the MT number, is matched to reaction names used by STAYSL PNNL via lookup tables that represent the information listed in Table 2. Cross section data is found by looking for the phrase "group constants at t=". If the associated MT number was requested (Table 2), then the subsequent data table of cross section information is extracted. Covariance data is found by looking for the phrase "relative covariance". If the MT number matches a requested reaction (Table 2), the subsequent table of covariances (if the values are not "zero") is read. If the covariances are for cross reactions, they are ignored unless the user requested them via the bCross parameter (see Table 3); cross reaction covariances are not requested for the purposes of STAYSL PNNL.

Based on the processing mode, data is written to the primary output file per the file structures described in Section 4.4.

4.5.1 Assumptions/Limitations

The following assumptions were used in the development of the NJpp code.

- The material/reaction pairs of interest are those defined in Table 2.
- The NJOY99 output is based on pointwise (or groupwise) reaction numbers (not those for metrology).
- When NJOY99 is run, the instructions for extracting cross sections/covariances from the IRDF-2002 library are grouped by material. That is, for each material there is a sequence of broadr, groupr, errorr (or possibly broadr, groupr, errorr, groupr, errorr), so that the data in the NJOY99 output file for a given material is consecutive.
- The same energy grid is used for all groupr and errorr instructions in the NJOY99 run directives input file (hence all data in the NJOY99 output file pertain to the same energy grid).
- The structure of the NJOY99 output file remains consistent (i.e., NJOY99 is not updated in such a way as to change the structure of the cross section or covariance output, nor the content of the key phrases used during parsing).
- The PNNL modifications are applied to NJOY99, whereby the errorr module writes covariances to the NJOY99 output file with more significant digits (see Section 3.1).

If the user specifies values for the M, N, and/or P parameters that, alone or in combination, are too large, then NJpp will terminate unsuccessfully, but gracefully, with an error message about insufficient memory. This should not be a problem typically, but may occur in special cases. Additionally, NJpp is limited to an energy grid of 699 groups (700 boundaries) when run in covariance processing mode because of the nature of the output file structure (a 2-dimensional matrix of data with all values in a row on one line).

NJpp relies on internal tables of reaction names (short and long), MAT numbers, and MT numbers. Any values other than those listed in Table 2 are ignored. However, should there be an attempt in the future to extract data for MT=1 (i.e., the [n, total] "reaction"), note that NJpp would fail due to the interspersed "flx" entries in the cross section table of the NJOY99 output.

5.0 SHIELD

5.1 Introduction/Background/Purpose

The SHIELD code calculates neutron self-shielding cross section correction factors that are used by the STAYSL PNNL code in the process of neutron spectral adjustment. The self-shielding factors are specific to a device (monitor sample) configuration (i.e., geometrical type and dimensions), the material of the device, and the flux type to which the device is exposed. Thus, the SHIELD code is run as needed, which may be infrequent if the same type of device is routinely used in the same type of flux environment.

SHIELD requires a library of cross sections, like STAYSL PNNL, but at a very fine energy grid resolution and for a select set of reactions. Non-threshold reactions (those with non-zero cross section data down to a neutron energy of 1×10^{-4} eV) are relevant to the self-shielding calculations performed by the SHIELD code. Self-shielding calculations are performed for flux monitor wire or foil dimensions and neutron flux environments (isotropic or beam) specified by the user. The SHIELD code produces a library of energy-dependent cross section correction factors that are used as input to STAYSL PNNL.

Application of SHIELD is contingent on assumptions about the cross sections and monitor sample size. Despite the use of a very fine energy grid for the neutron self-shielding calculations, the very fine resonance structure (represented in evaluated nuclear data files and accessible via a tool such as NJOY99) will not be accurately captured. However, such fine structure is not very important when considering the much broader neutron energy groups and the self-shielding corrections used during the neutron spectral adjustment performed by STAYSL PNNL. It is also recognized that the self-shielding equations for cylinders and plates are only applicable to flux monitor wires or foils that are relatively small because the equations do not account for neutron scattering or flux depression effects. If larger flux monitors are used (with thicknesses comparable to mean free path lengths for neutron scattering), then neutron transport codes such as MCNP [16, 17] are required to correctly account for neutron self-shielding effects.

5.2 Installing, Uninstalling, and Updating

SHIELD is a command line program that does not require any particular installation/uninstallation procedures per se on a Windows-based personal computer. The SHIELD code comes as a compiled executable file "shield.exe" that the user can simply place in any convenient directory. However, to execute the SHIELD code, the executable must be either located in the active directory from which it is being executed or it must be found in a directory in the command line window's search path. Section 3.2 describes the approaches to starting a command line program and how to modify the system search path (substitute SHIELD-specific information for path and executable, i.e., "shield.exe"). SHIELD can be uninstalled by deleting the "shield.exe" file and/or the associated program directory (e.g., "C:\Apps\SHIELD\"). If the user altered the standard search path, then the user should manually undo that change. SHIELD is updated simply by replacing the "shield.exe" file with a new file. The SHIELD version number and date are displayed when the code is run. See also Section 1.5 for information on automated installation and updates to the PATH environment variable.

5.3 Input Data and Run Options

SHIELD reads input from three files, two of which have fixed names and contain library data and the third of which contains the run option parameter values. Cross section data for a fine resolution energy grid (i.e., with a large number of energy groups) must be supplied in a file named "shldxsect.out." For the purposes of the STAYSL PNNL suite, the "shldxsect.out" file is generated by specifying input for NJOY99 pertaining to non-threshold reactions (as discussed in Section 3.3), running NJOY99, and then running NJpp (Section 4.0) on the resultant NJOY99 output. The other library type input file required must be named "shldengrp.dat" and needs to contain the energy grid boundaries for the coarse energy grid (that corresponds to the energy grid with fewer energy groups that will be analyzed with STAYSL PNNL). The "shldengrp.dat" file must have the data in the formatted structure described in Figure 10.

Record 1: <Number of energy group boundaries, MX>
Record 2: <Array of energy structure boundary values, in 7E11.4 format, in units of MeV>

Figure 10. *Structure of the "shldengrp.dat" file containing the energy grid for SHIELD output.*

The run parameters input file contains the data and options that determine the calculations for SHIELD to perform. The run parameters file name can be supplied as a command line argument when executing "shield.exe," or will be requested via an interactive prompt, and can be any convenient name. The run parameters input file has the structure described in Figure 11. The run parameters themselves are described in Table 4 and an example of the content of a run parameters input file is shown in Figure 12.

Record 1: <THK> <ATN>
Record 2: <sNameA> <2 spaces> <sWFvar> <1 space> <sTyp>
— Repeat records 1 & 2 for each device (or device variant) —

Figure 11. *Structure of the SHIELD run parameters input file.*

Table 4. *Description of SHIELD run option parameters.*

Input Parameter	Description & Constraints
THK	Thickness of foil or diameter of wire (mil), representing the mean chord
ATN	Atom density (atoms/cm³), which is a function of the sample density, alloy dilution factor (or abundance), Avogadro's constant, and atomic weight
sNameA	STAYSL PNNL short name for the reaction (Table 2); pad with spaces to have 6 characters total
sWFvar	Device variant name, user-define; pad with spaces to have 4 characters total; this value must also be used in the STAYSL PNNL run parameters input file because STAYSL PNNL searches for a match
sTYP	Type of device & flux (3-character string); must be one of these four options: BFX = 1 - Self-shielding for a foil with beam flux normal to the foil IFX = 2 - Self-shielding for a foil with isotropic flux BWX = 3 - Self-shielding for a wire with beam flux normal to the long axis IWX = 4 - Self-shielding for a wire with isotropic flux

```
20.0    7.97E+19
AU197G  AUAL IWX
20.0    9.09E+22
CO59G   CONG IWX
20.0    8.49e+22
FE58G   FENG IWX
```

Figure 12. *Example of a SHIELD run parameters input file for three monitor sample devices.*

5.4 Output

SHIELD produces two output files, one of which is the neutron self-shielding data library used as input to STAYSL PNNL and the other is annotated version of the same information. Both output files will have the same root file name as the run parameters input file, but the annotated file has a file extension of ".txt", while the data library output file has a file extension of ".out". The annotated text file includes the energy grid data and descriptive text, thus providing a user friendly file for diagnostic purposes. The data library file is the primary output from SHIELD, feeding directly into STAYSL PNNL as one of its input files. The structure of the data library output file is described in Figure 13, with several field names corresponding to run input parameters (Table 4) that are echoed back out.

Record 1: <sNameA> <2 spaces> <sTyp> <1 space> <THK (E10.3 format)> <Num. energy groups (I4 format)> <sWFvar>
Record 2: <Array of self-shielding data values, in 6ES14.7 format>
— Repeat records 1 & 2 for each device (or device variant) —

Figure 13. *Structure of the SHIELD output file.*

5.5 Calculations/Functionality

The SHIELD code implements the neutron self-shielding calculations for plates (i.e., foils) and cylinders (i.e., wires) for either an isotropic neutron flux or for a beam flux normal to the foil (or long axis of the wire). Chapter III of the IAEA's document on neutron fluence measurements [73] discusses neutron self-shielding for an isotropic flux of mono-energetic neutrons for plate and cylinder monitor sample geometries. Equations are presented for the general case as well as approximations for the case where the monitor sample (i.e., wire or foil) thickness is much less than the other dimensions. Additional equations are used to calculate the neutron self shielding for the scenario of a beam flux, based on basic principles of neutron absorption, as discussed below.

The self-absorption (self-shielding) factor of a sample, G, is the probability that the neutrons entering the sample will not be captured in it. In the case of a pure absorbing sample, each collision is a capture, so the self-absorption factor is $G = 1 - P_c$, where P_c is the collision probability.

Although the IAEA discussion of neutron self-shielding [73] notes that values for P_c have been tabulated by Placzek [74] for several geometries, it is more convenient to implement self-shielding equations that can be used for a wider variety of specific scenarios (geometry,

thickness, flux type, etc.). The equations used for the different categories of scenarios are described below. These self-shielding factor equations are formulated based on a dimensionless calculated parameter, *x*, which is equivalent to the thickness divided by the neutron absorption mean free path for a given reaction. The parameter *x* is calculated here (Equation 6) as the product of the microscopic cross section, σ (barns/atom), the material atom density, *ATN* (atom/cm^3), and the sample thickness, *THK* (mil). The latter two quantities are user inputs (see Section 5.3) and the former quantity is retrieved from the input data library (for a fine-resolution energy grid) that was assembled from the IRDF-2002 data file (Section 2.2) via NJOY99 (Section 3.0) and NJpp (Section 4.0). Note that *THK* is taken to be the mean chord of the sample, *a*, and the product $ATN \cdot \sigma$ corresponds to the macroscopic total cross section, Σ_t, which are the parameters discussed in the IAEA document [73].

$$x = THK \cdot ATN \cdot \sigma = a \cdot \Sigma_t \tag{6}$$

Consider neutron self-absorption for an infinite plate with an incident beam of neutrons normal to the surface of the plate. If we neglect neutron scattering, the relative self-absorption for transport a given distance into the plate is given by the exponential term e^{-x}, where *x* is defined in Equation 6 (and THK is replaced by the specific distance into the plate). The net absorption through a material of thickness *THK* is calculated by integrating this exponential term over the thickness of the plate, which results in Equation 7. If it is assumed that the finite sample is a foil whose thickness is much less than the other dimensions, then "end" effects can be neglected and Equation 7 is used to calculate the neutron self-absorption for a beam neutron flux. A similar derivation applies for the case of a foil exposed to an isotropic neutron flux, except that in this case the integration is over both the plate thickness and the range of all incident angles for the neutron flux. The neutron self-absorption in a thin foil for an isotropic neutron flux is given in Equation 8, which is equation III.34 from the IAEA document [73].

$$G_{foil,beam} = \frac{1 - e^{-x}}{x} \tag{7}$$

$$G_{foil,isotropic} = \frac{\frac{1}{2} - E_3(x)}{x} \tag{8}$$

The $E_3(x)$ term in Equation 8 represents the function for the third exponential integral, which can be calculated using polynomial/rational approximations from Abramowitz and Stegun (A&S) [58]. A&S equations 5.1.54 (for $x > 0$) and 5.1.53 (for $0 \le x \le 1$) can be combined with A&S equation 5.1.14 to obtain expressions for $E_3(x)$ for any positive value of *x*, as is shown in Equations 9 and 10 below.

$$E_3(x) = \frac{1}{2}\left\{e^{-x} - x\left[e^{-x}\left(1 - \frac{x^2 + 2.334733x + 0.250621}{x^2 + 3.330657x + 1.681534}\right)\right]\right\} \qquad 1 < x \qquad (9)$$

$$R = 0.00107857x^5 - 0.00976004x^4 + 0.05519968x^3 - 0.24991055x^2 + 0.99999193x - 0.57721566$$

$$E_3(x) = \frac{e^{-x} - xe^{-x} + x^2R - x^2\ln(x)}{2} \qquad 0 < x \le 1 \qquad (10)$$

Consider a cylinder of small diameter (radius = *r*) and infinite length with an incident beam of neutrons normal to the long axis of the cylinder (see cross section in Figure 14 on the next page). We can treat the cylinder as a stack of slices parallel to the incident neutron beam, where each slice has a "depth" of $2 \cdot r \cdot \sin(\theta)$ and a thickness of Δr (= $r \cdot \sin(\theta) \cdot \Delta\theta$). The neutron self absorption is then that for the slice "depth," integrated over all slices (applying symmetry to simplify the range of integration from 0° to 90°). If we assume that the wire (cylinder) length is much longer than its radius (such that end effects can be neglected), then this derivation leads to Equation 11 for a finite wire and a beam neutron flux. The derivation for a wire exposed to an isotropic neutron flux is similar, except that the integration is also over all possible angles of incidence. The neutron self-absorption in a wire for an isotropic neutron flux is given by Equation 12. These two equations carry out the integration as a sum of *numIter* number of finite thickness slices determined by the angle and a specified change in angle, $\Delta\theta$. Equations 14 and 13 describe *numIter* and $\Delta\theta$ (in radians), respectively. SHIELD uses a $\Delta\theta$ value of 0.1°, which equates to a *numIter* value of 900.

$$G_{wire,beam} = \left(\frac{4}{\pi \cdot x}\right) \cdot \left\{1.0 - \Delta\theta \cdot \sum_{i=1}^{numIter} \sin\left(\frac{\Delta\theta}{2} \cdot (2i-1)\right) \cdot e^{\left[-x \cdot \sin\left(\frac{\Delta\theta}{2} \cdot (2i-1)\right)\right]}\right\} \qquad (11)$$

$$G_{wire,isotropic} = \left(\frac{4}{\pi \cdot x}\right) \cdot \sum_{i=1}^{numIter} \Delta\theta \cdot \sin\left(\frac{\Delta\theta}{2} \cdot (2i-1)\right) \cdot \left\{\frac{1}{2} - E_3\left[x \cdot \sin\left(\frac{\Delta\theta}{2} \cdot (2i-1)\right)\right]\right\} \qquad (12)$$

$$numIter = \frac{90^\circ}{\Delta\theta_{degrees}} \qquad (13)$$

$$\Delta\theta = \Delta\theta_{degrees} \cdot \frac{\pi}{180^\circ} \qquad \text{(converting to radians)} \qquad (14)$$

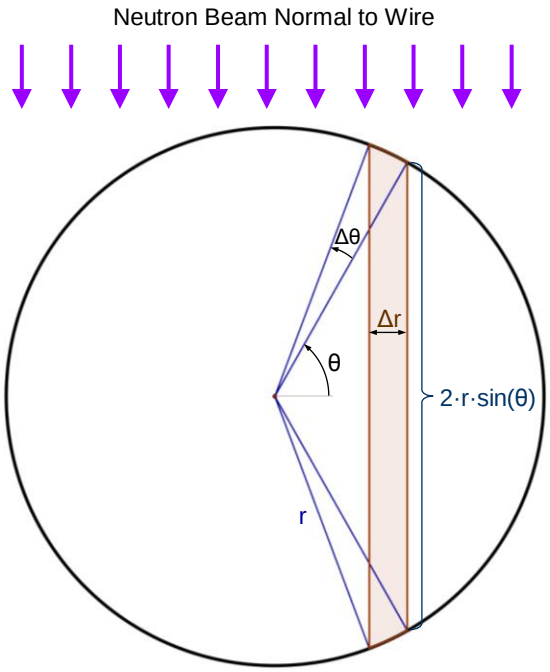


Figure 14. *Wire cross section.*

The self-shielding factor, G, is plotted in Figure 15, for the four combinations of neutron environment and sample device type.

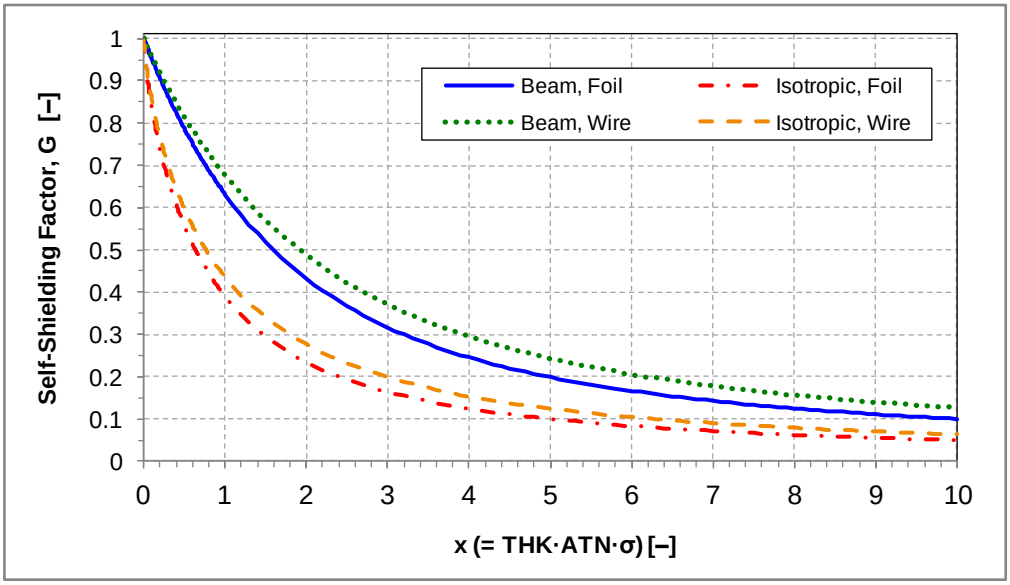


Figure 15. *Plot of the self-sheilding factor, G, as a function of the thickness/atom density/cross section parameter, x, for the four combinations of neutron environment (beam or isotropic) and sample device type (foil or wire).*

SHIELD calculates the self-shielding factors for each interval of the fine-resolution energy grid (i.e., the energy grid specified for non-threshold reactions, as discussed in Section 3.3), then collapses that information to a coarser user-specified energy grid (with a smaller number of energy groups) that will be used in STAYSL PNNL. To avoid inaccuracies introduced by partial overlap of energy grid intervals between the two grids, each of the boundaries of the coarse energy grid are required to align with a boundary of the fine-resolution energy grid (see Figure 16). However, the fine energy grid may span to a greater range above or below the extent of the coarse energy grid. Equation 15 is used to calculate the relative self-shielding factor, SSF_j, as the sum of the product of the cross section and the self-shielding factors for all fine grid intervals that are contained within a coarse grid interval, *j*, divided by the sum of the cross sections for those fine grid intervals. The *SSF* values are written to the SHIELD output with associated header information on reaction, monitor sample type, etc.

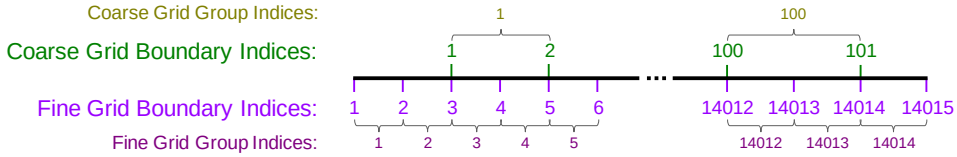


Figure 16. *Example of energy boundary alignment for the coarse energy grid to the fine energy grid, using boundary indices (not actual energies). Intervals between boundaries are the "energy groups" on which calculations are conducted.*

$$SSF_j = \frac{\sum_i G_i \cdot \sigma_i}{\sum_i \sigma_i} \qquad \text{i is summed over all fine grid intervals contained within the j}^{\text{th}} \text{ coarse grid interval} \qquad (15)$$

SHIELD guards against the situation where the reaction cross sections of all fine energy grid intervals within a single coarse energy grid interval sum to zero. If the sum of the cross sections in that coarse energy grid is zero, then, by definition, there is no neutron self-shielding because the probability of reaction is zero. If the sum of the cross sections is in the denominator of Equation 15 is zero for a given coarse energy grid interval, *j*, then the SHIELD code avoids a divide by zero error and simply sets SSF_j to 1.0 (i.e., no correction for neutron self-shielding).

5.5.1 Assumptions/Limitations

The following assumptions were used in the development of the SHIELD code.

- Very fine resonance structure has a minimal impact on the broader group neutron self-shielding corrections used during neutron spectral adjustment, thus the use of a very fine energy grid for the neutron self-shielding calculations is sufficient for approximating the self-shielding corrections.
- Neutron self-shielding is being calculated for relatively small flux monitor wires or foils where neutron scattering and flux depression effects are negligible.
- Available material/reaction pairs are those defined in Table 2, of which only the non-threshold reactions are pertinent to SHIELD.

- NJOY99 is used to extract cross section data for all Table 2 non-threshold reactions from the appropriate data source (i.e., IRDF-2002) and NJpp is used to reformat the extracted cross sections into a format suitable as an input library for SHIELD.
- A fine energy grid (e.g., 14015 grid boundary energies) is used in extracting cross sections data at a fine resolution from IRDF-2002, and this same grid is used for all groupr instructions in the NJOY99 run directives input file.
- Energy grid boundary data is provided in a monotonically increasing sequence.
- Self-shielding factors can be collapsed from the fine resolution energy grid to a coarse energy grid by summing up the contributions from the fine grid intervals that are contained within a given coarse grid interval.
- The coarse energy grid is encompassed by the range of the fine energy grid.
- If the calculated value of x (Equation 6) is less than 0.0001, then the self-shielding is assumed to be negligible and the self-shielding factor is set to 1.0.

As noted above in the discussion of the calculations performed by SHIELD and depicted in Figure 16, the energy grid boundaries for the coarse energy grid must all align with a boundary of the fine energy grid. If there is not alignment and the coarse energy grid is fixed, the only recourse is to regenerate the fine energy grid (i.e., with NJOY99 and NJpp) after inserting appropriate additional energy boundaries.

The SHIELD code only performs calculations for foil or wire type devices (monitor samples) in either a beam flux normal to the long axis or an isotropic flux. Other geometries would require determination of the neutron self-shielding factors via an alternate method.

The user is responsible for providing the input data specifying the mean chord (i.e., THK). There is no capability to calculate or select a mean chord based on monitor sample dimensions.

If flux monitors having a mean chord comparable to mean free paths for neutron scattering are used, then SHIELD should not be applied. Rather, neutron transport codes (e.g., MCNP [16, 17]) would be required to correctly account for neutron self-shielding effects because SHIELD does not account for neutron scattering or flux depression effects.

6.0 BCF

6.1 Introduction/Background/Purpose

The quantity of a radioactive isotope produced from a target material irradiated for a specified time in a nuclear reactor or at a particle accelerator depends on the detailed irradiation history. The calculation of the net activity at the end of irradiation must include corrections for production and decay during the irradiation event. Determining these corrections for irradiation at constant power is straightforward. However, in practice, the irradiation history may be quite complicated, with reactor power or accelerator beam current varying over time, including intervals of zero power. Furthermore, reactor irradiations may last for many years.

The purpose of the BCF code is to calculate the effective correction factor for each isotope of interest, normalized to the (time-weighted) average reactor power (or beam current). Dividing the power history into multiple sequential intervals of constant power, the effective correction factor is determined as the sum of the contributions to the activity for a specific isotope from each period of constant power, corrected for the decay during each given period and then decaying each contribution to the date when irradiation ended.

The BCF corrections are one component applied when calculating the "sig-phi" values (cross section times neutron flux [product atoms/target atoms/sec]). The output from the BCF code is used in the SigPhi Calculator spreadsheet software (see Section 7.0), which calculates the "sig-phi" values for subsequent use in the STAYSL PNNL code.

6.2 Installation, Uninstallation, and Updating

BCF is a command line program that does not require any particular installation/uninstallation procedures per se on a Windows-based personal computer. The BCF code comes as a compiled executable file "bcf.exe" that the user can simply place in any convenient directory. However, to execute the BCF code, the executable must be either located in the active directory from which it is being executed or it must be found in a directory in the command line window's search path. Section 3.2 describes the approaches to starting a command line program and how to modify the system search path (substitute BCF-specific information for path and executable, i.e., "bcf.exe").

BCF can be uninstalled simply by deleting the "bcf.exe" file and/or the associated program directory (e.g., "C:\Apps\BCF\"). If the user altered the standard search path, then the user should manually undo that change.

BCF is updated simply by replacing the "bcf.exe" file with a new file. The BCF version number and date are displayed when the code is run.

See also Section 1.5 for information on automated installation and updates to the PATH environment variable.

6.3 Input Data and Run Options

BCF reads input from two files, one of which has a fixed file name and contains library data for isotope half-lives and the other of which contains the run option parameter values.

The data library file is named "halflives.dat" and contains a list of isotopes, their associated half-lives, and identifiers for the half-life time units. The isotopes in the half-life library file correspond to the product isotopes listed in Table 2, which also lists the half-life values for each isotope. Half-lives may be specified in a variety of units, but, for consistency, the values in Table 2 (from Tuli [49]) are all specified in seconds. A decay constant may be specified instead of a half-life for an isotope, with the decay constant in the units of the irradiation data and a units flag value of "L." For consistency of downstream calculations (i.e., in SigPhi Calculator), nuclides representing stable products (e.g., 2-He-4) can be included. The half-life of a stable nuclide is represented as "--" (two dashes); see Section 6.5 (and Section 7.5) for discussion of calculations for stable nuclides. Table 5 describes the structure and the parameters of the "halflives.dat" file.

Table 5. *Structure of the nuclide data file (database) used by the BCF code.*

Record #	Variables	Fortran Format	# Repetitions	Description & Constraints
1	sNUCL, THLV, HUNIT	A10, G18.3, A1	multiple, no limit, repeat for each isotope of interest	sNUCL character string (10 characters maximum) specifying the name of the nuclide; the name must correspond with an item in the list in Table 2 (and thus in the SigPhi Calculator) THLV isotope-specific half-life or decay constant value; HUNIT determines whether THLV is a half-life or a decay constant; stable nuclides should list a half-life of two dashes ("--") HUNIT is a one-letter code for the time unit of the data. If HUNIT = "L," then THLV is a decay constant, which must be supplied in the same time units as the irradiation data (i.e., no internal conversion is done). Otherwise HUNIT may be one of the following characters indicating the time units of the half-life value: S (seconds), M (minutes), H (hours), D (days), Y (years)

The run parameters input file contains the data and options that determine the calculations for BCF to perform. The run parameters file name can be supplied as a command line argument when executing "bcf.exe," or will be requested via an interactive prompt, and can be any convenient name. Table 6 describes the structure of the run parameters input file and the meaning of the parameters, including valid options.

Irradiation time and FEE (i.e., neutron flux or other quantity proportional to the neutron flux) data must be provided in the run parameter input file for a sequence of constant FEE intervals, including intervals of zero flux (i.e., the sequence must explicitly include all intervals). The input run parameters NTYPE, NTIME, MFEE, and DUNIT are used to define the nature of the time and FEE data (i.e., cumulative or differential data, format of the time data, and whether the FEE is a rate or a total quantity).

Table 6. *Structure of the run parameters input data file for the BCF code.*

Record #	Variables	Fortran Format	# Repetitions	Description & Constraints
1	NTITL, NTYPE, NTIME, MFEE, DUNIT	4I2, A2	None	NTITL defines the number of title (annotation) lines. NTITL must be in the range 0 - 10 (inclusive). NTYPE defines the nature of the time & FEE data. NTYPE can take the following values: 0 differential time & differential FEE 1 differential time & cumulative FEE 2 cumulative time & differential FEE 3 cumulative time & cumulative FEE Differential means that distinct values are supplied for each time interval. Cumulative means that a running total is supplied, starting at the end of the first interval and assuming that time zero is a value of 0.0. Cumulative FEE values must be entered as fluence (or charge), thus MFEE must be 1 when NTYPE is 1 or 3. NTIME defines the format of the time data. NTIME can take the following values: 0 time, T, is a decimal value in the units specified by DUNIT 1 time is in same format as for NTIME = 0, but here the intervals are all the same duration (set by the single T value specified in record 4). NTYPE must be < 2 for this case. 2 time, T, is expressed as hours & minutes (or minutes & seconds) in a decimal format, where the integer portion is the number of hours (or minutes; the units are specified by DUNIT) and the fractional portion is the number of minutes (or seconds). E.g., 202.35 is 202 hours + 35 minutes. 3 time is in same format as for NTIME = 2, but here the intervals are all the same duration (set by the single T value specified in record 4). NTYPE must be < 2 for this case. MFEE defines whether the FEE data is a rate or not. MFEE can take the following values (see also notes above on NTYPE): 0 FEE is provided as a flux (or beam current), thus FEE is a rate (and no further conversion is needed). 1 FEE is provided as an integrated flux (defined as fluence) or integrated current (defined as charge), thus, FEE is a total quantity, not a rate. In this case, the code will convert FEE to a rate by dividing by the time interval duration. MFEE may be set to 1 regardless of the NTYPE value. DUNIT is a one letter code (in A2 format) for the time unit of the data: S = seconds, M = minutes, H = hours, D = days, Y = years. DUNIT must be either “H” or “M” when NTIME > 1.
2	TITLE	A80	NTITL times	Annotation text to describe the data set.
3	NREC	I10	None	Approximate number of lines of FEE/time data to be input. This number should be sufficiently large to encompass all data lines, including the end-of-data record, without being excessively large. E.g., a data set with 90 entries for record #4 could use NREC = 100.
4	T, FEE	* (free format)	NREC or fewer times	T duration of each interval in time units specified by DUNIT. If NTIME = 1 or = 3, then T must only be entered for the first <T><FEE> record; additional T values are not allowed. However, all NTYPE/NTIME cases require the last record (with FEE < 0.0) to include a T value that represents the total irradiation time (i.e., the sum of all the intervals). FEE reactor power or beam current for each interval. The end of the data is indicated by a negative FEE value in the last record of the run parameters input file.

Figure 17 depicts data for record 4 (Table 6) for the four possible permutations of NTYPE, given that NTIME = 0 and using the same root data. Cumulative data is always assumed to be relative to a "time zero" value of 0.0, thus a "time zero" value for cumulative must not be included in the list of data. If the actual cumulative data starts at a non-zero "time zero" value, then the user must externally convert the data to be relative to 0.0 at "time zero." The last record 4 entry consists of the total elapsed time and a negative FEE value to indicate that it is the end of the Time/FEE data. Figure 18 depicts data equivalent to that in Figure 17, but for a constant time interval. Examples of run parameter input file content are shown in Figure 19.

Repetition # of Rec. 4	Time Cumul.	FEE Cumul.	Time Diff.	FEE Diff.	Time Diff.	FEE Cumul.	Time Cumul.	FEE Diff.
1	36.0	900.0	36.0	25.0	36.0	900.0	36.0	25.0
2	42.0	900.0	6.0	0	6.0	900.0	42.0	0
3	84.0	2076.0	42.0	28.0	42.0	2076.0	84.0	28.0
4	96.0	2076.0	12.0	0	12.0	2076.0	96.0	0
5	114.0	2526.0	18.0	25.0	18.0	2526.0	114.0	25.0
6	120.0	2526.0	6.0	0	6.0	2526.0	120.0	0
7	156.0	3390.0	36.0	24.0	36.0	3390.0	156.0	24.0
8	156.0	-1	156.0	-1	156.0	-1	156.0	-1

Figure 17. *Comparison of lines of record 4 (Table 6) when time and FEE information (from the same root data set) are specified in various combinations of differential (D) and cumulative (C) values. Note that cumulative FEE is a total quantity, not a rate.*

diff Time	diff FEE
6	25
6	25
6	25
6	25
6	25
6	25
6	0
6	28
6	28
6	28
6	28
6	28
6	28
6	28
6	0
6	0
6	25
6	25
6	25
6	0
6	24
6	24
6	24
6	24
6	24
6	24

Figure 18. *Differential time and FEE data based on the same data set as in Figure 17, but with the time intervals all equal. A BCF run parameters input file would only include the first time value, leaving all other time values blank, and NTIME would be set to a value of 1 (constant time, decimal format) or 3 (constant time, clock format).*

```
 4 0 0 0 H
Reactor Irradiation from
  12/2/95 to 5/5/96
Example of diff. T,
  diff. FEE, decimal time
10
42.7    25
5.8     0
43.1    27
13.6    0
14.7    25
3       0
32      25
154.9   -1
```

```
 1 0 3 0 H
diff. T & FEE, clock time, equal time intervals
15
2.30   4
      18
      23
      26
      28
      31
      30
      30
      30
      28
      22
      14
       2
32.30 -1
```

Figure 19. *Examples of BCF run parameters input files with differential time and FEE (left) and with differential FEE and uniform equal differential time intervals (right). In the example on the right, note that for entries of record 4 after the first and before the end-of-data record, only the FEE value is included (do not include time data); these FEE values are right aligned for clarity in this example, but could be left aligned.*

The FEE parameter may refer to flux, fluence, current, charge, power, or some other quantity that is proportional to the neutron flux. It is the responsibility of the user to know what the FEE quantity represents and to track its units. Other than conversion from cumulative to differential, the BCF code does not track units or perform unit conversions on FEE. When the FEE data is presented as a set of cumulative values, the data must be as total quantity, not as rates.

6.4 Output

BCF produces two output files that are similar, with one file containing just the resultant data while the other file includes an echo of the input and additional annotations as well as the results. The annotated file is intended as a user friendly file for diagnostic purposes. The data output file is formatted for simple transfer en masse to a SigPhi Calculator worksheet for use as input information within that software (described in Section 7.0). Both output files will have the same root file name as the run parameters input file, but the annotated file has a file extension of ".txt", while the data output file has a file extension of ".out". A partial example of a data output file is depicted in Figure 20, showing a self-describing file structure (i.e., some labeled summary data followed by a table of data, including table headings).

```
      CAPT =   6.50000E+00 D       1.56000E+02 H
 CALC_CAPT =   6.50000E+00 D       1.56000E+02 H
     XPROD =   1.41250E+02 Qty×D   3.39000E+03 Qty×H
     AVGBM =   2.17308E+01 Qty

NUCLIDE     HALF-LIFE -    LAMBDA     EFF_FLUX      B_EFF     B_CONST   RATIO
(--)         (varies) (un)   (1/D)       (Qty)       (--)        (--)     (--)
2-He-4     Infinity   S  0.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00 1.000
9-F-18     6.5848E+03 S  9.0949E+00  2.4000E+01  1.1044E+00  1.0000E+00 1.104
11-Na-22   8.2135E+07 S  7.2914E-04  1.0274E-01  4.7279E-03  4.7282E-03 1.000
```

Figure 20. *Partial example of the content of a BCF data output file. A full file includes additional rows for other isotopes with the same types of data. The entire file is copied and pasted into a worksheet in the SigPhi Calculator to provide input for calculations in that software.*

The output data file includes summary and ancillary information as well as the primary value calculated by the BCF code. The CAPT is the actual elapsed time of the irradiation (including periods of zero power) based on the final entry for record 4 in the input file. The CALC_CAPT is a calculation of the actual irradiation time based on the sequence of time/FEE input data. The user can manually assess the CAPT and CALC_CAPT values to check that the input data was specified properly in the input file. The XPROD value is the "Integrated Flux-Time Product" (i.e., sum of time×FEE) and the AVGBM is the "Average Integrated Beam" (i.e., the time-weighted average neutron flux). The primary output data that is used in the SigPhi Calculator are the B_EFF values for each isotope, representing the flux history correction factors that are used to correct measured activities to saturation (decay corrected) activities. Data for EFF_FLUX (integrated corrected FEE values), B_CONST (flux history correction factor, assuming a constant irradiation), and RATIO (ratio of B_EFF to B_CONST) are included in the output for user convenience and potential diagnostics. For example, the ratio allows the user to assess the importance of the irradiation history for each nuclide.

6.5 Calculations/Functionality

The quantity of a radioactive isotope produced from a target material irradiated for a specified time in a nuclear reactor or at a particle accelerator depends on the detailed irradiation history. The calculation of the net activity at the end of irradiation must include corrections for production and decay during the irradiation event. For irradiation under constant conditions, the correction factor (also referred to as the "saturation factor" [38] or the "buildup of the nuclide during the irradiation period" [37]) for a specific isotope, $B_{const,\,j}$, is calculated with Equation 16.

$$B_{const,\,j} = 1 - e^{(-\lambda_j \cdot t)} \qquad \text{for the j}^{\text{th}}\text{ isotope} \qquad (16)$$

Here, λ_j is the isotope-specific decay constant (defined in Equation 17) for the jth isotope being produced, t is the total irradiation time, and $t_{½,\,j}$ is the half-life of the jth isotope being produced (Table 2).

$$\lambda_j = \frac{\ln(2)}{t_{½,\,j}} \qquad \text{for the j}^{\text{th}}\text{ isotope} \qquad (17)$$

In practice, the irradiation history may be quite complicated, with reactor power or accelerator beam current varying over time, including intervals of zero power. Furthermore, reactor irradiations may last for many years, much longer than the half-lives of the isotopes of interest.

The term "power" is used here to generically represent reactor power, reactor flux, reactor fluence, accelerator current, or accelerator charge. Any of these quantities are applicable. In the equations and the BCF output files, quantities are described as "flux" as a general term for a rate quantity. For a reactor irradiation event, the data that is available is generally the reactor power, which is nominally linearly proportional to the irradiation flux. Since the BCF code calculates dimensionless correction factors for each isotope of interest, "power" values can be entered as simple numbers or ratios rather than using absolute values. For example, a flux of 2.4×10^{12} n/cm^2-s can be entered as just 2.4 since the absolute normalization of the 10^{12} factor cancels out in all the equations. Power data can also be entered in terms of ratios to an average or maximum value. Consequently, it is the responsibility of the user to ensure that the "power" data is entered correctly and adequately represents the true variation of the time-dependent rate of production of the isotopes of interest.

The BCF code calculates the net correction for a variable irradiation history by using irradiation history data that is divided into intervals of constant power [38]. Such information is available from, for example, the reactor power history. Given multiple sequential intervals of constant power, the effective flux history correction factor, $B_{eff,j}$, can be calculated from Equation 18 (which also defines XPROD and AVGBM).

$$B_{eff,j} = \frac{\sum_{i=1}^{N} P_i \cdot \left[1 - e^{\left(-\lambda_j \cdot \Delta t_i\right)}\right] \cdot \left[e^{\left(-\lambda_j \cdot (t_e - t_{ie})\right)}\right]}{\sum_{i=1}^{N} \Delta t_i \cdot P_i \Big/ \sum_{i=1}^{N} \Delta t_i} = \frac{Effective\ Flux}{\left(XPROD \Big/ \Delta t_{tot}\right)} = \frac{Effective\ Flux}{AVGBM} \qquad \text{for the } j^{th} \text{ isotope} \qquad (18)$$

Here, P_i is the power for an irradiation interval, Δt_i is the duration of a given irradiation interval, Δt_{tot} is the total duration of irradiation, t_{ie} is the cumulative end time of a given irradiation interval, t_e is the cumulative end time at the end of the last interval, and N is the number of irradiation intervals. The contributions from each period of constant power are summed after correcting for the decay during the given period and then decaying this contribution to the date when irradiation ended, giving the effective flux. The effective flux is normalized to the (time-weighted) average power (AVGBM) to give the effective correction factor.

6.5.1 Assumptions/Limitations

The following assumptions were used in the development of the BCF code.

- If a decay constant is entered for a nuclide in the "halflives.dat" file, the time units are the same as for the irradiation data in the run parameters input file.
- The names of the nuclides in the "halflives.dat" file correspond with those in Table 2 for product isotopes.

- Reactor power is proportional to the irradiation flux and thus may be used as a surrogate for the irradiation flux (i.e., FEE). Similarly, other quantities may be used for the FEE values as long as they represent the actual variation of the time-dependent rate of production of the isotopes of interest. The FEE values need not be the absolute values, but they must be in the same proportions as the absolute values. This flexibility in type and magnitude of FEE value works because the correction factors are based on relative (i.e., normalized) values.
- The user has entered meaningful values for FEE and is cognizant of the units of measure, which will not be altered by the BCF code (other than to convert from a total quantity to a rate).
- Time or FEE data entered as cumulative values always assumes that the time zero value is 0.0, thus the time zero value does not need to be entered as an input.
- The corrections can be made by summing the decay-corrected contributions of multiple intervals of constant FEE.

The format specifications of the run input file (in particular the organization of the time and FEE data) must be properly followed based on the selected values of NTYPE, NTIME, and MFEE. Also, time or FEE input data that is specified on a cumulative basis must be monotonically increasing. When the FEE data is presented as a set of cumulative values, the data values must represent total quantity (e.g., fluence), not rates (e.g., flux).

No more than 10 lines of title information may be included in the run parameters input file.

If the absolute value of either exponent of the exponential terms in the numerator of Equation 18 exceeds a value of 180, then the exponent is constrained to a value of -180 to prevent underflow errors in the code.

7.0 SigPhi Calculator

7.1 Introduction/Background/Purpose

The purpose of the SigPhi Calculator software is to calculate corrected saturated neutron activation rates from measured activities. These reaction rates, the so-called "sig-phi" ($\sigma \cdot \phi$) values, represent the product of the spectral-averaged neutron activation cross section and the total neutron flux. The reaction rates are calculated from experimental activities measured for different samples and reactions by applying corrections for the irradiation history, gamma self-absorption (self-shielding), and neutron burn-up. The SigPhi Calculator applies the output from the BCF code (Section 6.0) to account for the production and decay over the timeframe of sample irradiation. Although, in certain instances, such as simple, short irradiations at constant reactor power or accelerator beam current, decay corrections can be included automatically via analytical equations in the gamma-ray spectrum analysis software and the BCF output is not required. Gamma self-absorption (self-shielding) corrections are calculated based on user-specified photon data and sample thickness. Neutron burn-up is calculated in the SigPhi Calculator based on irradiation event, reaction, and product isotope information. The SigPhi Calculator has the ability to account for neutron self-shielding (which must be included at some point to obtain meaningful results if such corrections are significant) as a simple numeric user input, but this feature should not be used because STAYSL PNNL applies the output of the SHIELD code to account for those effects. The main purpose of the SigPhi Calculator is to determine the saturated reaction rates (corrected sig-phi values) which are subsequently used as input to STAYSL PNNL for the spectral adjustment. An ancillary function of the SigPhi Calculator is to provide rough estimates of fast and thermal neutron fluences based on simplistic equations for the purpose of checking data consistency and to give the user an initial estimate for these fluences.

The SigPhi Calculator also acts as a repository for information (reaction names, half lives, MAT numbers, etc.) about reactions (and associated isotopes) processed by STAYSL PNNL. Data from this repository is used to manually configure input to the BCF, NJOY, SHIELD, and STAYSL PNNL codes.

7.2 Installing, Uninstalling, Updating, and Initiating the Software

The SigPhi Calculator software is implemented as a Microsoft Excel template workbook in Excel 97-2003 format (i.e., a "*.xlt" file) that can be used in Excel 2003 or Excel 2007 on a computer running Microsoft Windows XP or Windows 7 (other versions of Excel and Windows may also work, but are not specifically supported). Thus, installation consists of placing the template file into the appropriate directory (i.e., with a file manager utility or a save action), which makes the template automatically available from within Excel. Typical locations for templates are at the directory path "C:\Documents and Settings\ <username>\Application Data\Microsoft\Templates" for Windows XP and "C:\Users\<username>\AppData\Roaming\ Microsoft\Templates\" for Windows 7, where <username> is the user (login) name of the current

Windows user. A search of the hard drive or dialog boxes from within Excel may be helpful in determining the proper location for the template file on your particular system.

To uninstall the SigPhi Calculator, remove (move or delete) the template file from the "Templates" directory. This will remove it from the list of document templates in Excel.

See also Section 1.5 for information on automated installation of the template.

Each version of the SigPhi Calculator will have a unique filename (e.g., "SigPhi_Calculator_1.0.0.xlt") to identify the version of the template file (version information is also included on the main worksheet in the software). To update to a newer version, the new SigPhi Calculator template file is placed into the "Templates" directory. If desired, the old template file may be removed or deleted from the "Templates" directory. To update SigPhi Calculator calculations that were performed on a data set with a prior version of the SigPhi Calculator, the data from the old SigPhi Calculator workbook must be copied into a SigPhi Calculator workbook created from the new template file.

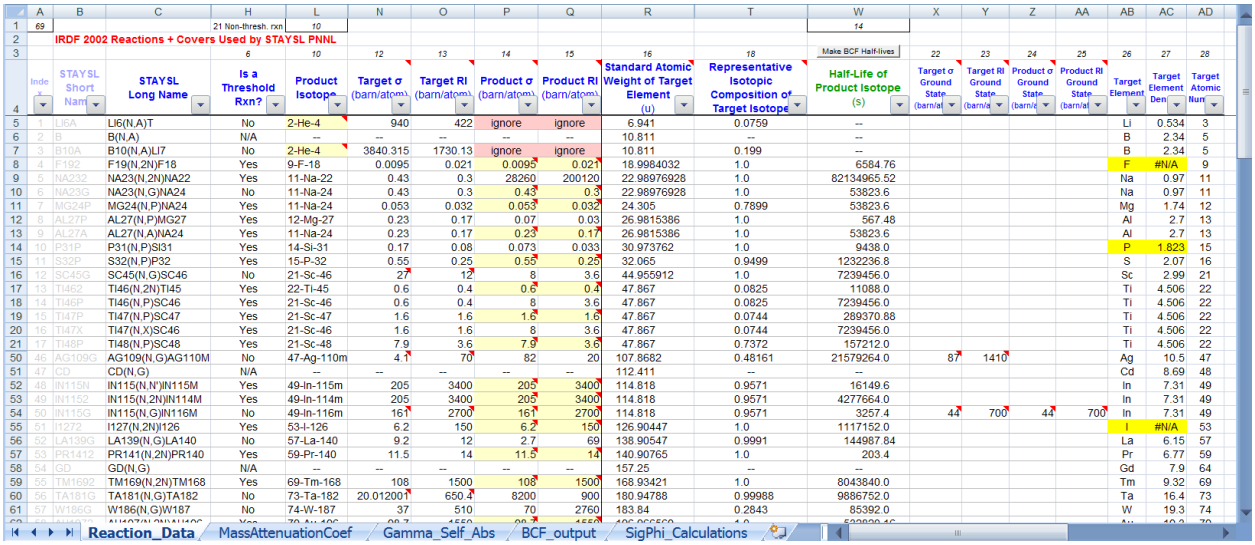
An "application run" with the SigPhi Calculator software is initiated by using the template file as the basis for a new Excel workbook. Use the File/New… (Excel 2003) or Office Button/New (Office 2007) menu item to select the current SigPhi Calculator template file and create a new workbook. This process results in an empty, unsaved, fully enabled document having a filename based on the template filename, but appended with an integer. The new document can be saved as a regular (i.e., non-template) Excel workbook (*.xls) and subsequently opened in the same manner as any other Excel workbook. When re-opening a saved SigPhi Calculator file in Excel, the user must enable macros for the software to work properly.

7.3 Software Interface, Input Data, and Run Options

The SigPhi Calculator software in an Excel workbook is comprised of five worksheets: Reaction_Data, MassAttenuationCoef, Gamma_Self_Abs, BCF_Output, and SigPhi_Calculations. These worksheets are described in this section, including items that are required as user inputs, options for the calculations, and actions that the user can take. The SigPhi Calculator workbook includes two features to help maintain the integrity of the calculations: the associated macro code is locked for viewing and the worksheets are protected, only allowing data entry in appropriate cells. Generally speaking, blue shading or font color indicates data input items, green shading/font indicates calculated values, a blue-green/aqua color is used to indicate optional user inputs (that have default values/calculations), an olive green/yellow is used to indicate where partial user input is required (with remaining values calculated), and a blue-gray color is used for optional inputs. Inline comments associated with column headings are provided to clarify user actions, parameter descriptions, and/or data sources.

The Reaction_Data worksheet (Figure 21) contains the information that is presented in Table 2 and acts as both a repository and a data input source. By default, only select columns are visible on Reaction_Data worksheet, reflecting that data which is pertinent to the SigPhi Calculator calculations (and, incidentally, to BCF). Inline comments describe the data sources (Section 2.1)

and assumptions. Rows 1 and 3 contain ancillary diagnostic/index numbers. If needed in the future, additional reactions could be added by inserting an entire row either in the middle of the table or immediately after the last row with data (although this addition would be done by the code custodian as part of the change request process). The "Make BCF Half-lives File" button on this worksheet is used to generate the data for the "halflives.dat" file that is used as input to the BCF code (see Section 6.3). When the "Make BCF Half-lives File" button is clicked, a formatted list of nuclide names and their half-lives is placed in the clipboard (copy) buffer. The user must then paste the information into an ASCII text file and save that file as "halflives.dat" into an appropriate directory.

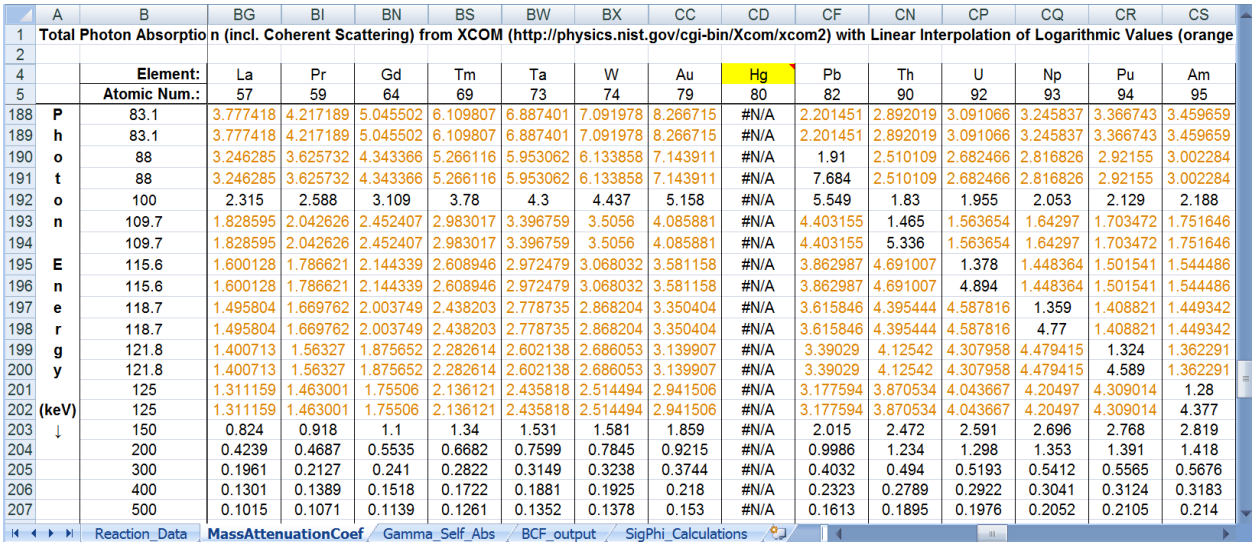


	A	B	C	H	L	N	O	P	Q	R	T	W	X	Y	Z	AA	AB	AC	AD
1	69			21 Non-thresh. rxn	10							14							
2	IRDF 2002 Reactions + Covers Used by STAYSL PNNL																		
3				6	10	12	13	14	15	16	18	Make BCF Half-lives	22	23	24	25	26	27	28
4	Index	STAYSL Short Name	STAYSL Long Name	Is a Threshold Rxn?	Product Isotope	Target σ (barn/atom)	Target RI (barn/atom)	Product σ (barn/atom)	Product RI (barn/atom)	Standard Atomic Weight of Target Element (u)	Representative Isotopic Composition of Target Isotope	Half-Life of Product Isotope (s)	Target σ Ground State (barn/a	Target RI Ground State (barn/a	Product σ Ground State (barn/a	Product RI Ground State (barn/a	Target Element	Target Element Den	Target Atomic Num
5	1	LI6A	LI6(N,A)T	No	2-He-4	940	422	ignore	ignore	6.941	0.0759	--					Li	0.534	3
6	2	B	B(N,A)	N/A	--	--	--	--	--	10.811	--	--					B	2.34	5
7	3	B10A	B10(N,A)LI7	No	2-He-4	3840.315	1730.13	ignore	ignore	10.811	0.199	--					B	2.34	5
8	4	F19Z	F19(N,2N)F18	Yes	9-F-18	0.0095	0.021	0.0095	0.021	18.9984032	1.0	6584.76					F	#N/A	9
9	5	NA23Z	NA23(N,2N)NA22	Yes	11-Na-22	0.43	0.3	28260	200120	22.98976928	1.0	82134965.52					Na	0.97	11
10	6	NA23G	NA23(N,G)NA24	No	11-Na-24	0.43	0.3	0.43	0.3	22.98976928	1.0	53823.6					Na	0.97	11
11	7	MG24P	MG24(N,P)NA24	Yes	11-Na-24	0.053	0.032	0.053	0.032	24.305	0.7899	53823.6					Mg	1.74	12
12	8	AL27P	AL27(N,P)MG27	Yes	12-Mg-27	0.23	0.17	0.07	0.03	26.9815386	1.0	567.48					Al	2.7	13
13	9	AL27A	AL27(N,A)NA24	Yes	11-Na-24	0.23	0.17	0.23	0.17	26.9815386	1.0	53823.6					Al	2.7	13
14	10	P31P	P31(N,P)SI31	Yes	14-Si-31	0.17	0.08	0.073	0.033	30.973762	1.0	9438.0					P	1.823	15
15	11	S32P	S32(N,P)P32	Yes	15-P-32	0.55	0.25	0.55	0.25	32.065	0.9499	1232236.8					S	2.07	16
16	12	SC45G	SC45(N,G)SC46	No	21-Sc-46	27	12	8	3.6	44.955912	1.0	7239456.0					Sc	2.99	21
17	13	TI46Z	TI46(N,2N)TI45	Yes	22-Ti-45	0.6	0.4	0.6	0.4	47.867	0.0825	11088.0					Ti	4.506	22
18	14	TI46P	TI46(N,P)SC46	Yes	21-Sc-46	0.6	0.4	8	3.6	47.867	0.0825	7239456.0					Ti	4.506	22
19	15	TI47P	TI47(N,P)SC47	Yes	21-Sc-47	1.6	1.6	1.6	1.6	47.867	0.0744	289370.88					Ti	4.506	22
20	16	TI47X	TI47(N,X)SC46	Yes	21-Sc-46	1.6	1.6	8	3.6	47.867	0.0744	7239456.0					Ti	4.506	22
21	17	TI48P	TI48(N,P)SC48	Yes	21-Sc-48	7.9	3.6	7.9	3.6	47.867	0.7372	157212.0					Ti	4.506	22
50	46	AG109G	AG109(N,G)AG110M	No	47-Ag-110m	4.1	70	82	20	107.8682	0.48161	21579264.0	87	1410			Ag	10.5	47
51	47	CD	CD(N,G)	N/A	--	--	--	--	--	112.411	--	--					Cd	8.69	48
52	48	IN115N	IN115(N,N')IN115M	Yes	49-In-115m	205	3400	205	3400	114.818	0.9571	16149.6					In	7.31	49
53	49	IN115Z	IN115(N,2N)IN114M	Yes	49-In-114m	205	3400	205	3400	114.818	0.9571	4277664.0					In	7.31	49
54	50	IN115G	IN115(N,G)IN116M	No	49-In-116m	161	2700	161	2700	114.818	0.9571	3257.4	44	700	44	700	In	7.31	49
55	51	I127Z	I127(N,2N)I126	Yes	53-I-126	6.2	150	6.2	150	126.90447	1.0	1117152.0					I	#N/A	53
56	52	LA139G	LA139(N,G)LA140	No	57-La-140	9.2	12	2.7	69	138.90547	0.9991	144987.84					La	6.15	57
57	53	PR141Z	PR141(N,2N)PR140	Yes	59-Pr-140	11.5	14	11.5	14	140.90765	1.0	203.4					Pr	6.77	59
58	54	GD	GD(N,G)	N/A	--	--	--	--	--	157.25	--	--					Gd	7.9	64
59	55	TM169Z	TM169(N,2N)TM168	Yes	69-Tm-168	108	1500	108	1500	168.93421	1.0	8043840.0					Tm	9.32	69
60	56	TA181G	TA181(N,G)TA182	No	73-Ta-182	20.01200	650.4	8200	900	180.94788	0.99988	9886752.0					Ta	16.4	73
61	57	W186G	W186(N,G)W187	No	74-W-187	37	510	70	2760	183.84	0.2843	85392.0					W	19.3	74

Reaction_Data | MassAttenuationCoef | Gamma_Self_Abs | BCF_output | SigPhi_Calculations

Figure 21. *Screen shot of part of the Reaction_Data worksheet in the SigPhi Calculator (additional rows have the same type of data for other reactions). The data in this table (including hidden columns) is that presented in Table 2. Only the visible columns shown here are pertinent to the SigPhi Calculator calculations. Numbers in rows 1 and 3 are ancillary diagnostic/index numbers. Shading of data and the associated inline comments describe data sources and assumptions.*

The MassAttenuationCoef worksheet (Figure 22) contains data for the linear mass attenuation coefficients, $\hat{\mu}$ (cm²/g), for pertinent elements based on the output from the XCOM database [55] maintained by the National Institute of Science and Technology. XCOM data was retrieved for each element of interest over a range of energies. This data (in a black font color) was subsequently aligned by energy and gaps were filled in with linear interpolation of logarithmic-transformed energy and $\hat{\mu}$ data (with results denoted by the orange font color). Further interpolation to a specific energy is performed on the SigPhi_Calculations worksheet. Some elements (e.g., F, I, Mg, Hg, etc.) are not used in gamma energy analysis or are only present as compounds (e.g., oxides), thus their mass attenuation coefficients are not applied. The user must manually determine the mass attenuation coefficients for alloys or compounds, as discussed in the Calculations section below.

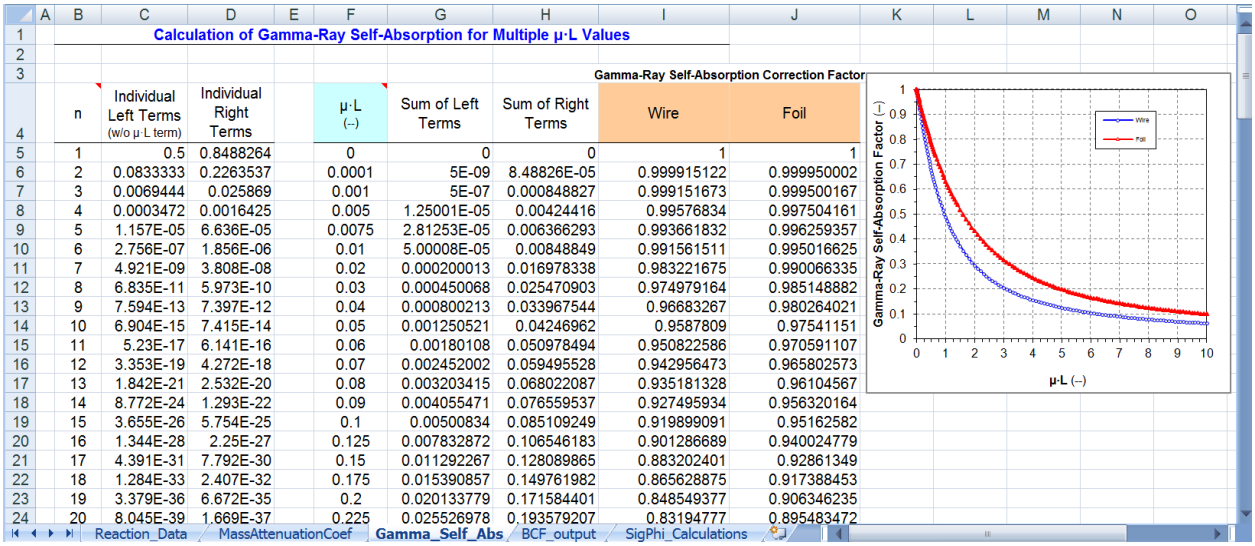


	A	B	BG	BI	BN	BS	BW	BX	CC	CD	CF	CN	CP	CQ	CR	CS
1	Total Photon Absorptio	n (incl. Coherent Scattering) from XCOM (http://physics.nist.gov/cgi-bin/Xcom/xcom2) with Linear Interpolation of Logarithmic Values (orange														
2																
4		Element:	La	Pr	Gd	Tm	Ta	W	Au	Hg	Pb	Th	U	Np	Pu	Am
5		Atomic Num.:	57	59	64	69	73	74	79	80	82	90	92	93	94	95
188	P	83.1	3.777418	4.217189	5.045502	6.109807	6.887401	7.091978	8.266715	#N/A	2.201451	2.892019	3.091066	3.245837	3.366743	3.459659
189	h	83.1	3.777418	4.217189	5.045502	6.109807	6.887401	7.091978	8.266715	#N/A	2.201451	2.892019	3.091066	3.245837	3.366743	3.459659
190	o	88	3.246285	3.625732	4.343366	5.266116	5.953062	6.133858	7.143911	#N/A	1.91	2.510109	2.682466	2.816826	2.92155	3.002284
191	t	88	3.246285	3.625732	4.343366	5.266116	5.953062	6.133858	7.143911	#N/A	7.684	2.510109	2.682466	2.816826	2.92155	3.002284
192	o	100	2.315	2.588	3.109	3.78	4.3	4.437	5.158	#N/A	5.549	1.83	1.955	2.053	2.129	2.188
193	n	109.7	1.828595	2.042626	2.452407	2.983017	3.396759	3.5056	4.085881	#N/A	4.403155	1.465	1.563654	1.64297	1.703472	1.751646
194		109.7	1.828595	2.042626	2.452407	2.983017	3.396759	3.5056	4.085881	#N/A	4.403155	5.336	1.563654	1.64297	1.703472	1.751646
195	E	115.6	1.600128	1.786621	2.144339	2.608946	2.972479	3.068032	3.581158	#N/A	3.862987	4.691007	1.378	1.448364	1.501541	1.544486
196	n	115.6	1.600128	1.786621	2.144339	2.608946	2.972479	3.068032	3.581158	#N/A	3.862987	4.691007	4.894	1.448364	1.501541	1.544486
197	e	118.7	1.495804	1.669762	2.003749	2.438203	2.778735	2.868204	3.350404	#N/A	3.615846	4.395444	4.587816	1.359	1.408821	1.449342
198	r	118.7	1.495804	1.669762	2.003749	2.438203	2.778735	2.868204	3.350404	#N/A	3.615846	4.395444	4.587816	4.77	1.408821	1.449342
199	g	121.8	1.400713	1.56327	1.875652	2.282614	2.602138	2.686053	3.139907	#N/A	3.39029	4.12542	4.307958	4.479415	1.324	1.362291
200	y	121.8	1.400713	1.56327	1.875652	2.282614	2.602138	2.686053	3.139907	#N/A	3.39029	4.12542	4.307958	4.479415	4.589	1.362291
201		125	1.311159	1.463001	1.75506	2.136121	2.435818	2.514494	2.941506	#N/A	3.177594	3.870534	4.043667	4.20497	4.309014	1.28
202	(keV)	125	1.311159	1.463001	1.75506	2.136121	2.435818	2.514494	2.941506	#N/A	3.177594	3.870534	4.043667	4.20497	4.309014	4.377
203	↓	150	0.824	0.918	1.1	1.34	1.531	1.581	1.859	#N/A	2.015	2.472	2.591	2.696	2.768	2.819
204		200	0.4239	0.4687	0.5535	0.6682	0.7599	0.7845	0.9215	#N/A	0.9986	1.234	1.298	1.353	1.391	1.418
205		300	0.1961	0.2127	0.241	0.2822	0.3149	0.3238	0.3744	#N/A	0.4032	0.494	0.5193	0.5412	0.5565	0.5676
206		400	0.1301	0.1389	0.1518	0.1722	0.1881	0.1925	0.218	#N/A	0.2323	0.2789	0.2922	0.3041	0.3124	0.3183
207		500	0.1015	0.1071	0.1139	0.1261	0.1352	0.1378	0.153	#N/A	0.1613	0.1895	0.1976	0.2052	0.2105	0.214

Reaction_Data | MassAttenuationCoef | Gamma_Self_Abs | BCF_output | SigPhi_Calculations

Figure 22. *Screen shot of part of the MassAttenuationCoef worksheet in the SigPhi Calculator (additional columns/rows have the same type of data for other elements/energies).*

The Gamma_Self_Abs worksheet (Figure 23) contains pre-calculated data pertaining to gamma self-absorption (self-shielding) correction factors. Gamma self-absorption is calculated as a function of the linear absorption coefficient (i.e., macroscopic absorption cross-section; product of density and linear mass absorption coefficient), μ, times the characteristic length (radius of a wire or thickness of a foil), L. Columns F through J on this worksheet contain calculations for gamma self-absorption in both wire and foil geometries for a list of specified $\mu \cdot L$ values, which provides data for the associated plot (right hand side of the worksheet in Figure 23). Although columns F through J could be used as a lookup table, the actual calculation of gamma self-absorption by the SigPhi Calculator is based on values of μ and L and the summation terms in columns C and D.

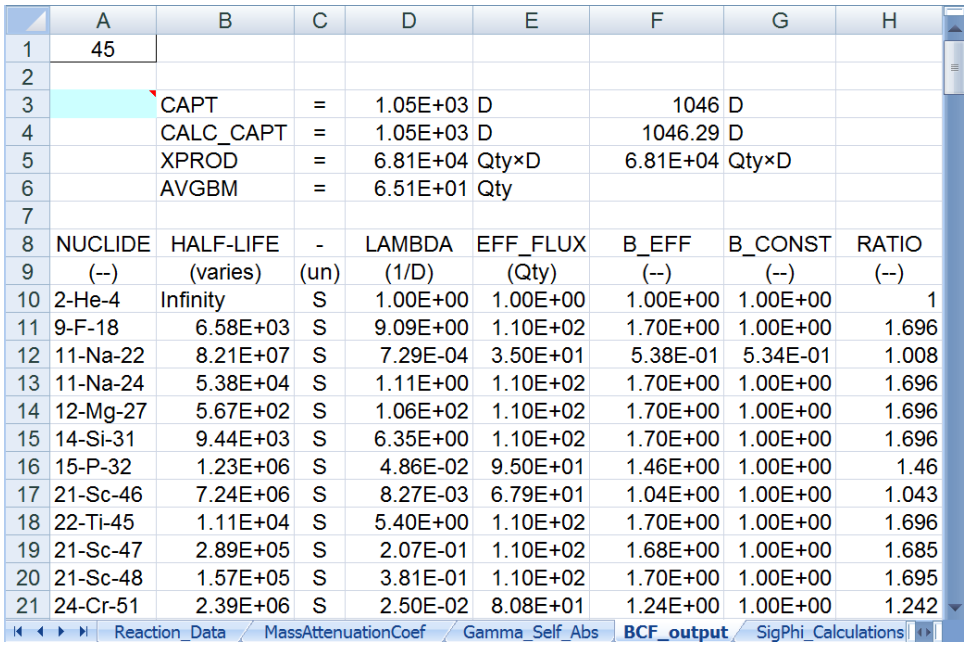


Calculation of Gamma-Ray Self-Absorption for Multiple μ·L Values

n	Individual Left Terms (w/o μ·L term)	Individual Right Terms	μ·L (--)	Sum of Left Terms	Sum of Right Terms	Gamma-Ray Self-Absorption Correction Factor: Wire	Foil
1	0.5	0.8488264	0	0	0	1	1
2	0.0833333	0.2263537	0.0001	5E-09	8.48826E-05	0.999915122	0.999950002
3	0.0069444	0.025869	0.001	5E-07	0.000848827	0.999151673	0.999500167
4	0.0003472	0.0016425	0.005	1.25001E-05	0.00424416	0.99576834	0.997504161
5	1.157E-05	6.636E-05	0.0075	2.81253E-05	0.006366293	0.993661832	0.996259357
6	2.756E-07	1.856E-06	0.01	5.00008E-05	0.00848849	0.991561511	0.995016625
7	4.921E-09	3.808E-08	0.02	0.000200013	0.016978338	0.983221675	0.990066335
8	6.835E-11	5.973E-10	0.03	0.000450068	0.025470903	0.974979164	0.985148882
9	7.594E-13	7.397E-12	0.04	0.000800213	0.033967544	0.96683267	0.980264021
10	6.904E-15	7.415E-14	0.05	0.001250521	0.04246962	0.9587809	0.97541151
11	5.23E-17	6.141E-16	0.06	0.00180108	0.050978494	0.950822586	0.970591107
12	3.353E-19	4.272E-18	0.07	0.002452002	0.059495528	0.942956473	0.965802573
13	1.842E-21	2.532E-20	0.08	0.003203415	0.068022087	0.935181328	0.96104567
14	8.772E-24	1.293E-22	0.09	0.004055471	0.076559537	0.927495934	0.956320164
15	3.655E-26	5.754E-25	0.1	0.00500834	0.085109249	0.919899091	0.95162582
16	1.344E-28	2.25E-27	0.125	0.007832872	0.106546183	0.901286689	0.940024779
17	4.391E-31	7.792E-30	0.15	0.011292267	0.128089865	0.883202401	0.92861349
18	1.284E-33	2.407E-32	0.175	0.015390857	0.149761982	0.865628875	0.917388453
19	3.379E-36	6.672E-35	0.2	0.020133779	0.171584401	0.848549377	0.906346235
20	8.045E-39	1.669E-37	0.225	0.025526978	0.193579207	0.83194777	0.895483472

Figure 23. *Screen shot of part of the Gamma_Self_Abs worksheet in the SigPhi Calculator (additional rows have the same type of data for subsequent values of n and μ·L). Columns F through J and the plot are for information only, providing examples of the calculations over a range of μ·L values.*

The BCF_Output worksheet is used to hold the data produced by the BCF code (Section 6.0). This worksheet is initially blank except for cells A1 (a diagnostic calculation) and A3. The user must copy the contents of the BCF data output file (Section 6.4) from a text file editor, select the shaded cell A3 on the BCF_Output worksheet, and paste the file contents into the worksheet. The user must then use Excel's "Text to Columns" functionality to parse the text as delimited data with a space delimiter. This will result in data in columns A through H, as the example in Figure 24 shows. If the "Text to Columns" functionality had been used previously, the user may need to reset the delimiters (if a conflicting delimiter was previously specified) or may not need to do any further processing (if the space delimiter had been previously specified). The parsed output from the BCF code provides information (XPROD, AVGBM, B_EFF) specific to a particular irradiation event that is used in the SigPhi Calculator calculations.



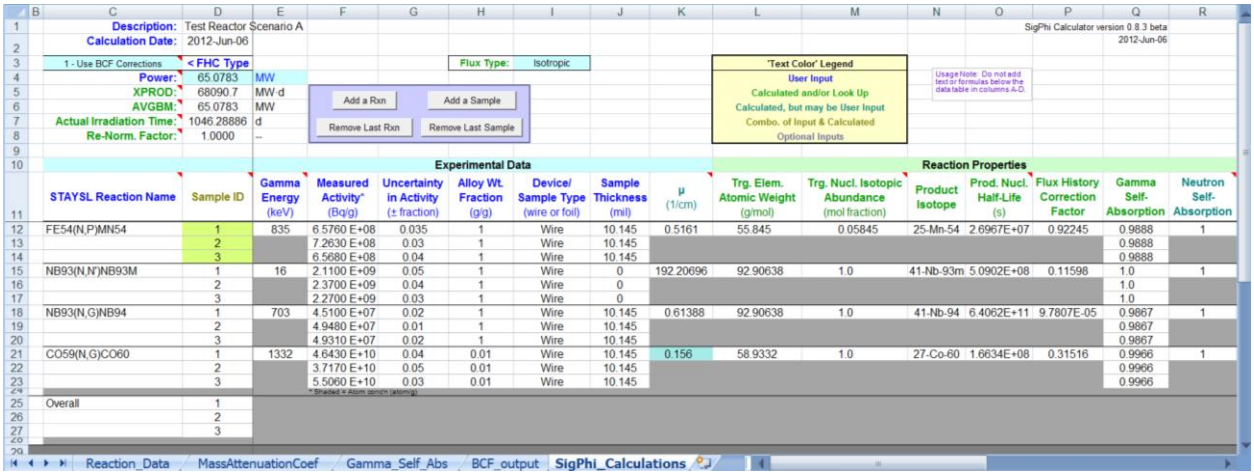
	A	B	C	D	E	F	G	H
1	45							
2								
3		CAPT	=	1.05E+03	D	1046	D	
4		CALC_CAPT	=	1.05E+03	D	1046.29	D	
5		XPROD	=	6.81E+04	Qty×D	6.81E+04	Qty×D	
6		AVGBM	=	6.51E+01	Qty			
7								
8	NUCLIDE	HALF-LIFE	-	LAMBDA	EFF_FLUX	B_EFF	B_CONST	RATIO
9	(--)	(varies)	(un)	(1/D)	(Qty)	(--)	(--)	(--)
10	2-He-4	Infinity	S	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1
11	9-F-18	6.58E+03	S	9.09E+00	1.10E+02	1.70E+00	1.00E+00	1.696
12	11-Na-22	8.21E+07	S	7.29E-04	3.50E+01	5.38E-01	5.34E-01	1.008
13	11-Na-24	5.38E+04	S	1.11E+00	1.10E+02	1.70E+00	1.00E+00	1.696
14	12-Mg-27	5.67E+02	S	1.06E+02	1.10E+02	1.70E+00	1.00E+00	1.696
15	14-Si-31	9.44E+03	S	6.35E+00	1.10E+02	1.70E+00	1.00E+00	1.696
16	15-P-32	1.23E+06	S	4.86E-02	9.50E+01	1.46E+00	1.00E+00	1.46
17	21-Sc-46	7.24E+06	S	8.27E-03	6.79E+01	1.04E+00	1.00E+00	1.043
18	22-Ti-45	1.11E+04	S	5.40E+00	1.10E+02	1.70E+00	1.00E+00	1.696
19	21-Sc-47	2.89E+05	S	2.07E-01	1.10E+02	1.68E+00	1.00E+00	1.685
20	21-Sc-48	1.57E+05	S	3.81E-01	1.10E+02	1.70E+00	1.00E+00	1.695
21	24-Cr-51	2.39E+06	S	2.50E-02	8.08E+01	1.24E+00	1.00E+00	1.242

Reaction_Data | MassAttenuationCoef | Gamma_Self_Abs | **BCF_output** | SigPhi_Calculations

Figure 24. *Screen shot of part of an example BCF_Output worksheet in the SigPhi Calculator (additional rows have the same type of data for other nuclides).*

The SigPhi_Calculations worksheet is the main location for user interaction and data input (the BCF_Output worksheet will be used routinely to input the BCF code data; the other three worksheets generally will not be visited). The SigPhi_Calculations worksheet contains multiple zones for data entry or types of calculations and is basically split into two halves. The left half of the SigPhi_Calculations worksheet (Figure 25) includes an area for general information in the upper left, a set of buttons for managing the number of reactions and samples that are to be assessed in the calculation, a section for entering experimental data, and a section where reaction properties are calculated based on the experimental data and the table of reaction/isotope data in the Reaction_Data worksheet. Moving further to the right in the SigPhi_Calculations worksheet (Figure 26), there is an area where intermediate calculations are performed and the final corrected sig-phi results determined. Further right still in the worksheet are rough calculations for the fluence (neutrons/cm^2) for fast and thermal neutrons based on user input for cross sections and estimates of the ratio of epithermal to thermal fluence.

The user must enter several types of data on SigPhi_Calculations worksheet, the first block of which are the annotation and general parameters in the upper left portion of the worksheet. For calculation annotation purposes, the user is asked for a description of the irradiation/data set and the date of the calculation. The user must also specify the nature of neutron flux (irradiation) history corrections ("FHC Type") as being based on the BCF code or as having been applied already by via gamma-ray spectrum analysis software. The approach can be selected via the drop-down list in cell C3. If the irradiation history corrections come from the BCF code, the user merely needs to specify the magnitude of the "power," *P*, in units that are consistent with the FEE data used in the BCF code (as discussed in Section 6.3); other parameters are

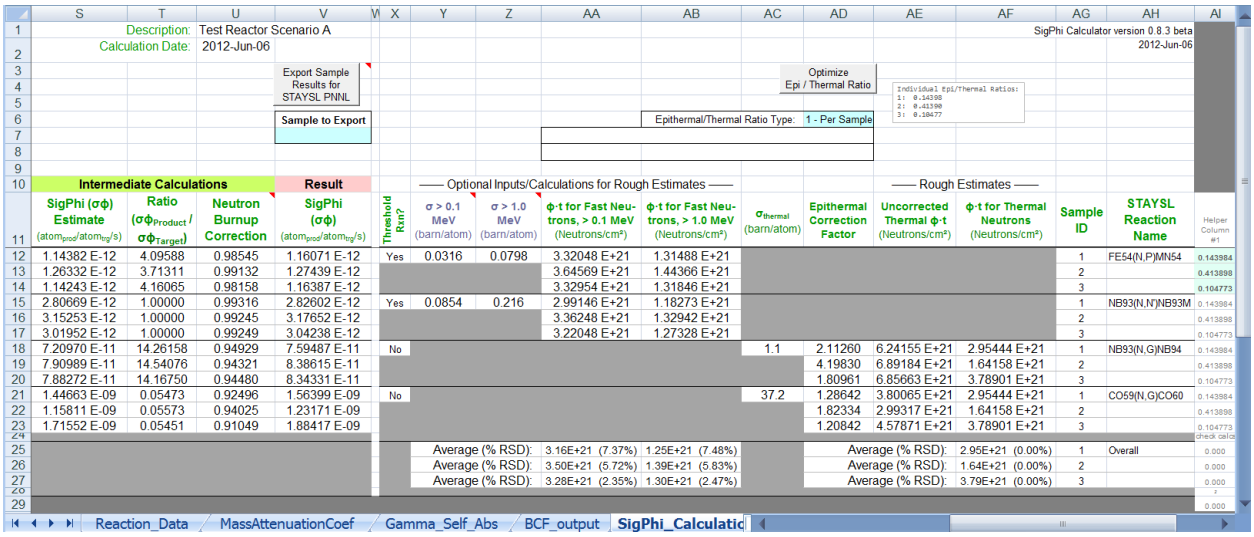


Description:	Test Reactor Scenario A														SigPhi Calculator version 0.8.3 beta		
Calculation Date:	2012-Jun-06														2012-Jun-06		
1 - Use BCF Corrections	< FHC Type				Flux Type:	Isotropic			'Text Color' Legend								
Power:	65.0783	MW							User Input								
XPROD:	68090.7	MW-d	Add a Rxn	Add a Sample					Calculated and/or Look Up								
AVGBM:	65.0783	MW							Calculated, but may be User Input								
Actual Irradiation Time:	1046.28886	d	Remove Last Rxn	Remove Last Sample					Combo. of Input & Calculated								
Re-Norm. Factor:	1.0000	--							Optional Inputs								

		Experimental Data								Reaction Properties						
STAYSL Reaction Name	Sample ID	Gamma Energy (keV)	Measured Activity* (Bq/g)	Uncertainty in Activity (± fraction)	Alloy Wt. Fraction (g/g)	Device/ Sample Type (wire or foil)	Sample Thickness (mil)	μ (1/cm)	Trg. Elem. Atomic Weight (g/mol)	Trg. Nucl. Isotopic Abundance (mol fraction)	Product Isotope	Prod. Nucl. Half-Life (s)	Flux History Correction Factor	Gamma Self-Absorption	Neutron Self-Absorption
FE54(N,P)MN54	1	835	6.5760 E+08	0.035	1	Wire	10.145	0.5161	55.845	0.05845	25-Mn-54	2.6967E+07	0.92245	0.9888	1
	2		7.2630 E+08	0.03	1	Wire	10.145							0.9888	
	3		6.5680 E+08	0.04	1	Wire	10.145							0.9888	
NB93(N,N')NB93M	1	16	2.1100 E+09	0.05	1	Wire	0	192.20696	92.90638	1.0	41-Nb-93m	5.0902E+08	0.11598	1.0	1
	2		2.3700 E+09	0.04	1	Wire	0							1.0	
	3		2.2700 E+09	0.03	1	Wire	0							1.0	
NB93(N,G)NB94	1	703	4.5100 E+07	0.02	1	Wire	10.145	0.61388	92.90638	1.0	41-Nb-94	6.4062E+11	9.7807E-05	0.9867	1
	2		4.9480 E+07	0.01	1	Wire	10.145							0.9867	
	3		4.9310 E+07	0.02	1	Wire	10.145							0.9867	
CO59(N,G)CO60	1	1332	4.6430 E+10	0.04	0.01	Wire	10.145	0.156	58.9332	1.0	27-Co-60	1.6634E+08	0.31516	0.9966	1
	2		3.7170 E+10	0.05	0.01	Wire	10.145							0.9966	
	3		5.5060 E+10	0.03	0.01	Wire	10.145							0.9966	
Overall	1														
	2														
	3														

Reaction_Data | MassAttenuationCoef | Gamma_Self_Abs | BCF_output | SigPhi_Calculations

Figure 25. *Screen shot of the leftmost part of the main SigPhi_Calculations worksheet (containing example data) in the SigPhi Calculator.*



Description:	Test Reactor Scenario A														SigPhi Calculator version 0.8.3 beta		
Calculation Date:	2012-Jun-06														2012-Jun-06		
			Export Sample Results for STAYSL PNNL								Optimize Epi / Thermal Ratio						
			Sample to Export						Epithermal/Thermal Ratio Type:	1 - Per Sample							

Intermediate Calculations			Result		Optional Inputs/Calculations for Rough Estimates						Rough Estimates					
SigPhi (σφ) Estimate (atom$_{prod}$/atom$_{trg}$/s)	Ratio (σφ$_{Product}$ / σφ$_{Target}$)	Neutron Burnup Correction	SigPhi (σφ) (atom$_{prod}$/atom$_{trg}$/s)	Threshold Rxn?	σ > 0.1 MeV (barn/atom)	σ > 1.0 MeV (barn/atom)	φ·t for Fast Neutrons, > 0.1 MeV (Neutrons/cm²)	φ·t for Fast Neutrons, > 1.0 MeV (Neutrons/cm²)	σ$_{thermal}$ (barn/atom)	Epithermal Correction Factor	Uncorrected Thermal φ·t (Neutrons/cm²)	φ·t for Thermal Neutrons (Neutrons/cm²)	Sample ID	STAYSL Reaction Name	Helper Column #1
1.14382 E-12	4.09588	0.98545	1.16071 E-12	Yes	0.0316	0.0798	3.32048 E+21	1.31488 E+21					1	FE54(N,P)MN54	0.143984
1.26332 E-12	3.71311	0.99132	1.27439 E-12				3.64569 E+21	1.44366 E+21					2		0.413898
1.14243 E-12	4.16065	0.98158	1.16387 E-12				3.32954 E+21	1.31846 E+21					3		0.104773
2.80669 E-12	1.00000	0.99316	2.82602 E-12	Yes	0.0854	0.216	2.99146 E+21	1.18273 E+21					1	NB93(N,N')NB93M	0.143984
3.15253 E-12	1.00000	0.99245	3.17652 E-12				3.36248 E+21	1.32942 E+21					2		0.413898
3.01952 E-12	1.00000	0.99249	3.04238 E-12				3.22048 E+21	1.27328 E+21					3		0.104773
7.20970 E-11	14.26158	0.94929	7.59487 E-11	No					1.1	2.11260	6.24155 E+21	2.95444 E+21	1	NB93(N,G)NB94	0.143984
7.90989 E-11	14.54076	0.94321	8.38615 E-11							4.19830	6.89184 E+21	1.64158 E+21	2		0.413898
7.88272 E-11	14.16750	0.94480	8.34331 E-11							1.80961	6.85663 E+21	3.78901 E+21	3		0.104773
1.44663 E-09	0.05473	0.92496	1.56399 E-09	No					37.2	1.28642	3.80065 E+21	2.95444 E+21	1	CO59(N,G)CO60	0.143984
1.15811 E-09	0.05573	0.94025	1.23171 E-09							1.82334	2.99317 E+21	1.64158 E+21	2		0.413898
1.71552 E-09	0.05451	0.91049	1.88417 E-09							1.20842	4.57871 E+21	3.78901 E+21	3		0.104773
					Average (% RSD):		3.16E+21 (7.37%)	1.25E+21 (7.48%)			Average (% RSD):	2.95E+21 (0.00%)	1	Overall	0.000
					Average (% RSD):		3.50E+21 (5.72%)	1.39E+21 (5.83%)			Average (% RSD):	1.64E+21 (0.00%)	2		0.000
					Average (% RSD):		3.28E+21 (2.35%)	1.30E+21 (2.47%)			Average (% RSD):	3.79E+21 (0.00%)	3		0.000

Reaction_Data | MassAttenuationCoef | Gamma_Self_Abs | BCF_output | SigPhi_Calculatic

Figure 26. *Screen shot of the rightmost part of the main SigPhi_Calculations worksheet (containing example data) in the SigPhi Calculator.*

determined from the BCF code output that is placed on the BCF_Output worksheet as described above. If gamma-ray spectrum analysis software was used to process data, then the user must enter information for the irradiation time, the renormalization factor (RNF), and the magnitude/ units of *P* (which is simply annotation in this case, and thus optional). The formatting of the items in the range C4:E8 of the SigPhi_Calculations worksheet alters according to the approach selected for irradiation history corrections to reflect whether the parameters are user inputs, calculated values, or not needed. In cell I3, the user should select the type of neutron flux field (isotropic or beam) from the drop-down list; this information is used when exporting the results.

If results from the BCF code are used, then the user-specified power in the SigPhi Calculator determines the nature of the time and the value of the renormalization factor (calculations are

described in Section 7.5). If the user applies the power calculated by the BCF code (i.e., AVGBM), then the time represents the actual irradiation time (including downtime) and no renormalization is applied (RNF = 1.0). If the user specifies a different value for power (which must be greater than AVGBM), then it is assumed that the user has specified "full power" and therefore the time represents the effective full power time (and thus the renormalization factor will be greater than 1.0). The calculated sig-phi values are directly impacted by the approach to time/power via the renormalization factor. However, neutron fluence values (and the product of the sig-phi values and the time, though these values are not calculated or reported by the software) are unaffected by the normalization approach. See Section 1.3 and Figure 7 for discussion of the relationship between flux, time, and fluence.

The main data entry takes place on the SigPhi_Calculations worksheet starting at row 12, below the row of headings, in columns C through K. Data is organized by one or more samples for each of a set of reactions. The user must first configure the worksheet with the proper number of reactions and samples using the four buttons in the cell range of F5:H8 to add or remove (increase or decrease) the number of samples and/or reactions. The same samples are assumed to apply to all reactions, so the user only needs to specify sample identifiers for the first reaction in column D (the names are automatically displayed for all other reactions). Reaction names should be entered on just the first row of each subgroup in the positions indicated. The main gamma energy and the μ values are also specified once per reaction. Measured activity, the fractional relative uncertainty for the activity, alloy weight fraction, device (sample) type, and characteristic length (L) are entered for every sample of every reaction. The sample type is limited to choices of "Wire" or "Foil." The characteristic length value corresponds to the radius of a wire or thickness of a foil. If the sample consists of material dissolved in solution and deposited on a surface (such as might be used for niobium-93 on an X-ray mount), then the user should specify the sample as a "Foil" and either use the very small actual thickness to account for the tiny amount of gamma absorption or specify a thickness of 0.0 to simply neglect gamma absorption. If a "Wire" is specified with L = 0.0, gamma absorption will be neglected, but that would tend to be a confusing way to document the situation. Also note that the characteristic length should be consistent with SHIELD data (although SHIELD uses wire diameter, whereas SigPhi Calculator wants wire radius).

An optional data entry location is present towards the right side of the SigPhi_Calculations worksheet in columns Y and Z, where cross section values can be entered for threshold (non-thermal) reactions. Cross sections for energies both greater than 0.1 MeV and greater than 1.0 MeV, can be provided for each threshold reaction. These cross sections should represent the best estimate available to the user because these values solely determine the reliability of the fast neutron fluence estimates. Ideally, the cross sections should be average values from the neutron spectrum. If an initial representation of the neutron flux spectrum is available (which is an input to STAYSL PNNL), then the user can perform a STAYSL PNNL FIR run (i.e., without spectral adjustment) to obtain cumulative integral flux values, from which spectral averaged cross sections can be determined. If the neutron spectrum is not known, then a first cut at fast neutron cross sections could be to adopt values from the U-235 fission spectrum (such as are tabulated in

Table 6.1 of the IRDF-2002 documentation [5]) or to estimate cross section values based on neutron cross section plots or tables of evaluated nuclear data files.

An estimate of the ratio of epithermal to thermal fluences is required. There are two approaches to an estimate for this ratio: have one overall ratio (for all reactions and all samples) or have one ratio per sample (that applies to all reactions for that sample). The approach can be selected using the drop-down list in cell AD6. The estimate(s) for the ratio can be either entered manually (in cell AD7 or in column AI starting at row 12) or the user can request that the SigPhi Calculator try to determine an appropriate ratio. To have the software automatically estimate the ratio(s), click on the "Optimize Epi/Thermal Ratio" button. The automated process of determining the epithermal/thermal fluence performs an optimization search with the objective of minimizing the relative standard deviation of the rough estimates for the thermal neutron fluences.

An average thermal neutron fluence value is needed to estimate the burn-up correction factor. If there are no thermal (non-threshold) reactions being assessed in the current data set, then the user needs to specify an average thermal neutron fluence in cell AD8.

Once the data inputs are provided, the calculations proceed automatically to apply the correction factors to the sig-phi values. If data is missing, error values will appear or results will be blank. It is possible to omit specific measured activity data (i.e., for one sample) and the calculations will proceed (although the automated optimization of the epithermal/thermal ratio could possibly fail to complete, depending on how many reactions there are).

7.4 Output

There are two outcomes from the calculations performed by the SigPhi Calculator software. The main results are the corrected reaction rate (sig-phi) values in column V, which are subsequently used as input to STAYSL PNNL for the spectral adjustment process. Although the user could manually transfer the calculated sig-phi values to record 5 of the STAYSL PNNL run parameters input file, the semi-automated process is recommended to ensure consistency. The user can select the sample identifier of interest (to export) from the drop-down list in cell V7 and then click the "Export Sample Results for STAYSL PNNL" button. This will place the appropriate data (properly formatted) for all reactions for that sample into the clipboard (copy) buffer. The exported data includes not only the short reaction names and the sig-phi values needed for STAYSL PNNL record 5, but also the KG and KA values for record 2 as well as the TIME and ACNM values for record 4. The user can manually paste the data into the ASCII text STAYSL PNNL run parameters input file (see Section 8.3). When using this button to copy data, placeholders (of numbers or repeated letters, with appropriate decimals and spaces) are included for the remaining fields of each input data record. Figure 27 shows an example of the information sent to the copy buffer with the "Export Sample Results for STAYSL PNNL" button. It is strongly recommended that the user not adjust either of the exported TIME or ACNM values, thus ensuring that the STAYSL PNNL run is consistent with the calculated sig-

phi values from the SigPhi Calculator. If a change in time basis is desired, it is straightforward to adjust the SigPhi Calculator inputs and export the updated results for a STAYSL PNNL run.

```
### Set options in Records 2-3; All but KG, KA, TIME, & ACNM are placeholders ###   DELETE THIS LINE
Test Reactor Scenario A
  100    4    1    0    1     <-- KG    KA    IPNT  IACT  KQT  (5I5)
0.005  9.0  0.03  0.03        <-- ACVX  FCHN  FCVX  FS         (free format)
0.0   0   0  90399357.1  1.0  <-- AK1   NORML ILOG  TIME  ACNM (free fmt: R,I,I,R,R)
FE54P    1.144E-12 0.035                       IWX
NB93N    2.807E-12 0.050                       IWX
NB93G    7.595E-11 0.020                       IWX
CO59G    1.564E-09 0.040                       IWX
nnnnnnnnSSSSSSSSS a.aaa COVR bb.bb SHLD cc.cc IWX  < for fmt. ref. only; DELETE THIS LINE
Activity Covariance Annotation goes on this line (if ACVX <0)
Put Activity Covariance Data Matrix here in free format if ACVX <0
Flux Uncertainty Annotation goes on this line if IACT = 0
NGP (I4 format)
Flux Uncertainty Data Matrices go here in free format as either just FCOV or as EIN followed by FCIN
Flux Covariance Annotation goes on this line if IACT = 1 and FCHN <= 0
Flux Covariance Matrix goes here in free format if IACT = 1 and FCHN <= 0
Input Flux Spectrum Annotation goes on this line
NGP, ITHERM, TNORM, TMPR, ETE  (2I4, 3F10.4 format)
Input Flux Spectrum Data Matrices go here in free format as either just F or as EIN followed by FIN
10 Element array of Number of Groups per bin goes here in free format
```

Figure 27. *Example of data put into a copy buffer from the SigPhi Calculator for transfer (pasting) into a STAYSL PNNL run parameters input file. Note that the default value of 0.03 used for FS will likely need to be manually changed to a value more like 0.001.*

An ancillary function of the SigPhi Calculator is to provide rough estimates of fast and thermal neutron fluences, which is the second outcome of the spreadsheet calculations. These neutron fluence values are simple estimates and are only provided as a convenience to the user for checking data consistency and as a preliminary estimate. As noted above, these simple estimates of fluence values are only as reliable as the spectral-averaged cross section estimates. The user really needs to run STAYSL PNNL to get the most reliable estimates of the neutron fluence values.

7.5 Calculations

The calculations necessary to determine correction factors and the corrected reaction rates are described in this section. Several overall parameter values are calculated first, followed by correction factors for the irradiation history, gamma self absorption, neutron burn-up, which all contribute to the final calculation of the corrected reaction rate. Additional calculations are used to estimate fast and thermal neutron fluences (Section 7.5.1).

In general, it is recommended that the user apply the BCF code for all flux history corrections. Indeed, the BCF code is the only applicable approach when assessing longer irradiations where the neutron flux (i.e., reactor power or beam current) varies over time. For simple, short irradiations at constant reactor power or accelerator beam current, it is possible to correct for decay during irradiation in some gamma-ray spectrum analysis software packages, such as

Genie™ 2000[1] [75, 76] or SAMPO[2] [77]. Therefore, the corrections calculated by the BCF code (Section 6.0) would not be required. Gamma-ray spectrum analysis software will commonly report the saturation (decay corrected) activities (i.e., the activity after an infinite irradiation time) and often offer the option to correct for decay during sample collection time (e.g., for air filters). Saturation activities from the gamma-ray spectrum analysis software do not require any further adjustment. However, activities that include a correction for sample collection time, must have that correction "backed out" to obtain the saturation activities. These variants of corrections applied within gamma-ray spectrum analysis software are referred to as "Saturation Activity" and "Saturation Activity with Sampling Decay" flux history correction types. To provide the necessary corrections, the user must select the appropriate flux history type in the SigPhi Calculator, whether that is to use corrections determined with the BCF code or one of the calculational variants of the gamma-ray spectrum analysis software.

As discussed in Section 7.3, the selected nature of neutron flux (irradiation) history corrections impacts whether several values are user inputs or calculated. When the BCF code is used and its output data is placed on the BCF_Output worksheet, the *XPROD* and *AVGBM* parameter values (discussed in Section 6.5) are taken directly from the BCF output data (although the time units of *XPROD* are converted to days, if not already in days). Additionally, the irradiation time, T_{irr}, and the renormalization factor, *RNF*, are calculated from *XPROD*, *AVGBM*, and the user-specified "power," *P*, using Equations 19 and 20, respectively. If the specified power is greater than the *AVGBM* value (it cannot be less than *AVGBM*), then it is assumed that the irradiation time is the effective full power time (otherwise the time is assumed to be the actual irradiation time).

$$T_{irr} = \frac{XPROD}{P} \tag{19}$$

$$RNF = \frac{P}{AVGBM} \tag{20}$$

If gamma-ray spectrum analysis software was used in acquiring/processing the activity measurements, then the irradiation time, T_{irr}, and renormalization factor, *RNF*, are user inputs. If the user enters a *RNF* value that is greater than 1.0, then the irradiation time is assumed to be the effective full power time (hence the actual irradiation time, including downtime, would be $RNF \cdot T_{irr}$). The *XPROD* and *AVGBM* parameters are not used in this case.

The neutron flux history correction factor, *FHCF*, is calculated based on the user-specified "FHC Type." When using the BCF code, the *FHCF* value is just the B_EFF value (Equation 21) that the BCF code calculated (see Section 6.5, Equation 18, and Figure 20). The selection of either gamma-ray spectrum analysis software option for the "FHC Type" implies that corrections for a short duration, constant neutron flux irradiation have already been applied. In the "Saturation

[1] Genie is a trademark of Canberra Industries, Inc.
[2] SAMPO is a trademark of Logion Oy.

Activity" case, it is assumed that the simple flux history correction factor described by Equation 16 (e.g., equation 203 of the Genie 2000 manual [76] or equation 9.25 of the SAMPO manual [77]) has been applied. Thus, *FHCF* is set to 1.0 (Equation 22), because no further correction is required in this case. The "Saturation Activity with Sampling Decay" case includes the correction factor of Equation 16 as well as an additional correction factor for decay during sample collection (e.g., equation 201 of the Genie 2000 manual [76] or equation 9.26 of the SAMPO manual [77]). This additional term must be "backed out" of the activity value calculated by the gamma-ray spectrum analysis software, which is accomplished by setting *FHCF* to the reciprocal of this term (Equation 23, where $t_{½,\,product}$ is the product nuclide half-life in seconds, and the 86400 is a conversion factor from days to seconds).

$$FHCF = B\_EFF \qquad \text{FHC Type = Use the BCF code} \qquad (21)$$

$$FHCF = 1.0 \qquad \text{FHC Type = "Saturation Activity"} \qquad (22)$$

$$FHCF = \frac{\ln(2) \cdot RNF \cdot T_{irr} \cdot 86400}{t_{1/2,\,product}} \qquad \text{FHC Type = "Sat. Act. w/ Sampl. Decay"} \qquad (23)$$

The gamma self-absorption correction factor, *GSA*, is calculated as a function of the linear absorption coefficient (i.e., macroscopic absorption cross-section), μ, times the characteristic length (radius of a wire or thickness of a foil), *L* (whose product is defined in Equation 24 for clarity). The absorption coefficient can be calculated with Equation 25 using the absorption cross section (σ_{target}), density (ρ_{target}), and atomic mass (MW_{target}) of the target nuclide. N_A is Avogadro's constant (equal to 6.02214129×10^{23} atom/mol [57]). Absorption cross section data can be found in the literature (e.g., [78]) and need to be converted to length units consistent with the density and characteristic length parameter. Alternately, the linear mass attenuation coefficient, $\hat{\mu}$, can be obtained from the literature [55] and multiplied times density to obtain μ (Equation 25). As noted in Section 7.3, the SigPhi Calculator applies this latter approach, assuming that the sample is a pure material. If the sample contains impurities or compounds, the user must manually apply Equation 25 in a summation of the mass attenuation coefficients for all elements present along with the appropriate density [79]. For a foil (planar) sample, the gamma self-absorption is calculated by the simple formula in Equation 26 (e.g., equation 2-15 of Greenberg et al. [80]). Calculation of gamma self-absorption for a sample with wire (cylindrical) geometry is based on a series expansion to an arbitrary (but rigorous) 50 terms, as shown in Equation 27. The summation in Equation 22 shown here applies the assumptions that the sample is of small radius and that the distance to the detector is much greater than this sample radius to Equations 22 and 23 of Evans and Evans [81].

$$s_i = (\mu \cdot L)_i \qquad \text{for the i}^{th}\text{ reaction; L = wire radius or foil thickness} \qquad (24)$$

$$\mu_{target} = \frac{\sigma_{target} \cdot N_A \cdot \rho_{target}}{MW_{target}} = \hat{\mu}_{target} \cdot \rho_{target} \qquad \text{for the target nuclide of the i}^{th}\text{ reaction (for pure materials)} \qquad (25)$$

$$GSA_i = \frac{1 - e^{-s_i}}{s_i} \qquad \text{for the i}^{th}\text{ reaction and Foil geometry} \qquad (26)$$

$$GSA_i = 1 + \sum_{n=1}^{50} \left[\frac{1}{n!\,(n+1)!} \cdot s_i^{2n} - \frac{16^n\ n!\,(n-1)!}{\pi\ (2n-1)!\,(2n+1)!} \cdot s_i^{2n-1} \right] \qquad \text{for the i}^{\text{th}} \text{ reaction and Wire geometry} \quad (27)$$

For the purposes of the STAYSL PNNL software suite, neutron self-absorption (self-shielding), *NSA*, is determined via the SHIELD code (Section 5.0) and applied directly within STAYSL PNNL. The SigPhi Calculator features an option to include calculations for neutron self-absorption, but this should be left unchanged at the default value of 1.0.

An initial estimate of the sig-phi, $\sigma\phi_{initial}$, value can be calculated for each reaction and sample based on the measured activity, $\hat{A}$, the correction factors described above, the user-specified alloy weight fraction, *AWF*, and tabulated data for the target nuclide. In the case of the LI6A and B10A reactions, the quantity, *Q*, of a product (here 2-He-4, in atoms/g) is measured instead of an activity (units of Bq/g). To place the quantity of product on the same basis as the activity values, *Q* must be divided by T_{irr}, as shown in Equation 28 The calculation for $\sigma\phi_{initial}$ is shown in Equation 29 (see ASTM documents [35, 38, 34, 13, 37] for related discussion), where $Abund_{target}$ is the isotopic abundance for the target nuclide (other parameters have been previously defined).

$$A_{i,j} = \hat{A}_{i,j} \qquad \text{for the j}^{\text{th}} \text{ sample of the i}^{\text{th}} \text{ reaction where activity (Bq/g) is measured}$$

$$or \qquad (28)$$

$$A_{i,j} = \frac{Q_{i,j}}{T_{irr} \cdot 86400} = \frac{Q_{i,j}}{t} \qquad \text{for the j}^{\text{th}} \text{ sample of the i}^{\text{th}} \text{ reaction where quantity (atom/g) is measured}$$

$$\sigma\phi_{initial,i,j} = \frac{A_{i,j} \cdot RNF \cdot MW_{target,i}}{FHCF_i \cdot GSA_i \cdot NSA_i \cdot AWF_{i,j} \cdot Abund_{target,i} \cdot N_A} \qquad \text{for the j}^{\text{th}} \text{ sample of the i}^{\text{th}} \text{ reaction} \quad (29)$$

An estimate of the ratio of epithermal to thermal fluences, $r_{epi:therm}$, is required to calculate the neutron burn-up. As explained in Section 7.3, the user may arrive at this ratio either by using optimization methods included as part of the SigPhi Calculator software or by manually specifying the value(s) as user input. The $r_{epi:therm}$ ratio can be specified as one overall number for all reactions and samples or as a set of numbers that are specific to a sample. In the equations below, this ratio is assumed to be sample-specific, but an overall number without subscript indices could also be used. The $r_{epi:therm}$ ratio is used in the ancillary calculations (Section 7.5.1), where the basis for automated optimization ($\Phi_{thermal}$) is described.

The ratio of the product nuclide reaction rate, $\sigma\phi_{product}$, to the target nuclide reaction rate, $\sigma\phi_{target}$, is defined to be r_{sp} and is calculated from the cross sections, σ, and resonance integrals, *RI*, of the respective nuclides in the reaction (listed in Table 2) as well as the ground state cross sections, σ_{GS}, and ground state resonance integrals, RI_{GS} (noted in Table 2 footnotes). The calculation of r_{sp} is shown in Equation 30. If the cross section of the product, $\sigma_{product}$, is undefined, as is the case for the 3-Li-6 (N,A) and the 5-B-10 (N,A) reactions, then r_{sp} is also undefined.

$$rNumer = \sigma_{GS,product,i} + \sigma_{product,i} + (RI_{GS,product,i} + RI_{product,i}) \cdot r_{epi:therm,j}$$

$$rDenom = \sigma_{GS,target,i} + \sigma_{target,i} + (RI_{GS,target,i} + RI_{target,i}) \cdot r_{epi:therm,j} \quad \text{for the j}^{th}\text{ sample of the i}^{th}\text{ reaction} \quad (30)$$

$$r_{sp,i,j} = \frac{rNumer}{rDenom}$$

Neutron burn-up calculations (discussed by IAEA [5] and ASTM [35]) are performed for each reaction and sample to determine the burn-up correction factor, *NBU* via a user-defined function (i.e., an Excel "macro") that provides the capabilities of the BURNS/BURNUP codes (see Section 1.2). This function encapsulates the algorithm shown in Figure 28, whose outcome depends on the nature of the input. For non-threshold (thermal) reactions (with two exceptions discussed below) the algorithm iterates to find an estimate that meets a specific tolerance. For threshold (fast) reactions, the algorithm does not iterate and simply exits after calculating the burn-up correction factor. As shown in Equation 31, the burn-up correction for thermal reactions is based on the initial sig-phi estimate for the reaction, while the burn-up correction for fast reactions is based on an average thermal sig-phi (which is discussed at the end of Section 7.5.1 with respect to Equation 40). Along with the $\sigma\phi_{burnup}$, the previously described quantities of T_{irr}, *RNF*, r_{sp}, and λ (from Equations 19, 20, 30, and 17, respectively) are used in Equation 32 within the algorithm to calculate *NBU*. Equation 32 effectively represents a ratio of cases with and without burn-up. Note that $t = T_{irr} \cdot 86400\ ^{s}/_{day}$ (to convert irradiation time to seconds).

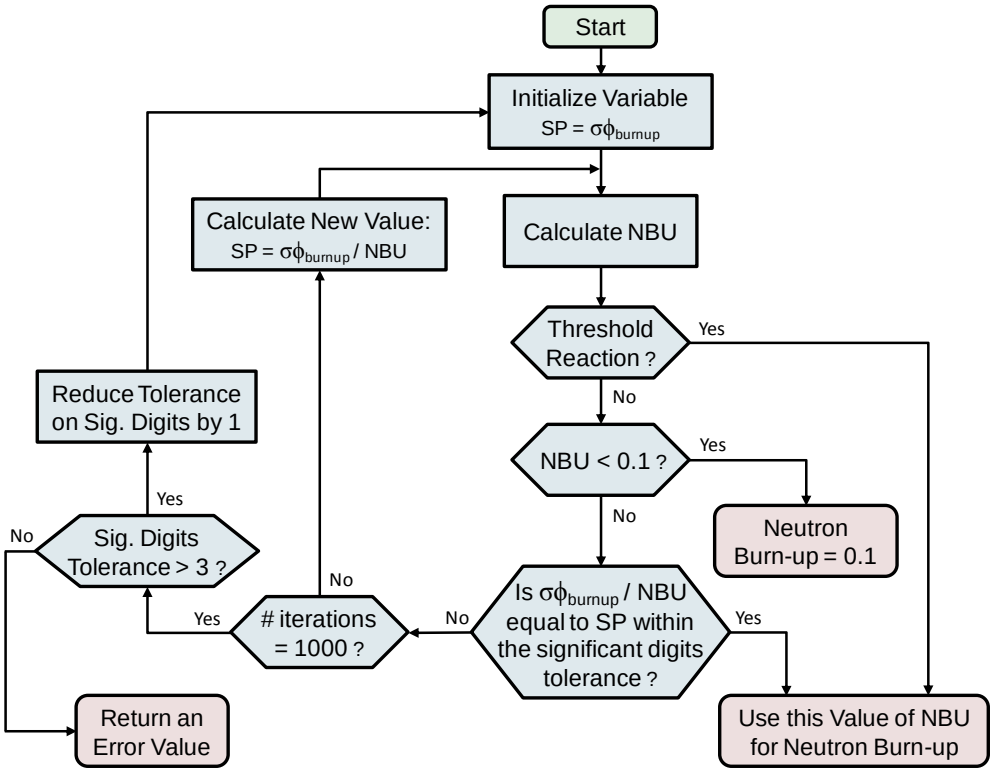


Figure 28. *Algorithm for the NeutronBurnup( ) user-defined function in the SigPhi Calculator to arrive at the neutron burn-up correction factor. The "Calculate NBU" step applies Equation 32 or Equation 33.*

$$\sigma\phi_{burnup\,i,j} = \sigma\phi_{initial,i,j}$$ for the j[th] sample of the i[th] non-threshold (thermal) reaction

or (31)

$$\sigma\phi_{burnup\,i,j} = \sigma\phi_{avg\_thermal,i,j}$$ for the j[th] sample of the i[th] threshold (fast) reaction (see also Equation 40)

$$NBU_{i,j} = \frac{RNF \cdot \lambda_i \cdot \left[e^{-SP_{i,j} \cdot t} - e^{\left(-t \cdot (RNF \cdot \lambda_i + SP_{i,j} \cdot r_{sp,i,j})\right)}\right]}{\left[RNF \cdot \lambda_i + SP_{i,j} \cdot \left(r_{sp,i,j} - 1\right)\right] \cdot \left[1 - e^{-RNF \cdot \lambda_i \cdot t}\right]}$$ for the j[th] sample of the i[th] reaction. The $SP_{i,j}$ variable is defined in Figure 28 (32)

Convergence of the iterative process in Figure 28 is based on estimates of the *SP* value being equal to the burn-up-corrected sig-phi value out to a specified number of significant digits (initially, 7 digits). The algorithm assumes that 1000 iterations will be sufficient to converge on a result, but will reduce the convergence tolerance incrementally (to no less than 3 digits) and re-check the iteration, then fails with an error if convergence isn't achieved at less stringent tolerances. To avoid calculational overflow, if the iteration reaches a *NBU* value less than 0.1, then the function exits and uses 0.1 as the burn-up factor. When this limit is reached, the burn-up factor is highlighted in the spreadsheet with light red shading to indicate that there may be issues with the reaction for the particular flux history scenario and that the burn-up may be too large for the SigPhi Calculator to suitably calculate a sig-phi value. If $\sigma\phi_{burnup}$ equals 0.0 (or is blank/absent), then *NBU* is simply set to 1.0 without ever applying the algorithm. Note that the use of *RNF* in Equation 32 corrects the time to actual irradiation time (versus effective full power time) to properly account for decay.

The LI6A and B10A thermal reactions are special cases with respect to burn-up due to the large cross sections of the targets and the correspondingly high burn-up involved. Additionally, the measured product (2-He-4) is stable (infinite half-life) and has effectively zero cross section (which means that $r_{sp} = 0$). Hence, these two reactions are treated as threshold (fast) reactions for the purpose of estimating burn-up. The burn-up correction factor is calculated non-iteratively using a simplified equation (Equation 33) in place of Equation 32.

$$NBU_{i,j} = e^{-SP_{i,j} \cdot t}$$ for the j[th] sample of the i[th] reaction (which must be either the LI6A reaction or the B10A reaction) (33)

Once the burn-up correction factor is determined, the primary output of the SigPhi Calculator software, $\sigma\phi$, is calculated using Equation 34.

$$SigPhi_{i,j} = \sigma\phi_{i,j} = \frac{\sigma\phi_{initial,i,j}}{NBU_{i,j}}$$ for the j[th] sample of the i[th] reaction (34)

7.5.1 Ancillary Calculations

As a user convenience, the SigPhi Calculator also performs ancillary calculations to give a preliminary indication of data consistency by using simplistic equations for fast, Φ_{fast}, and thermal, $\Phi_{thermal}$, neutron fluences (where fluence, in units of neutrons/cm², is the product of the

average neutron flux, ϕ, and the irradiation time, T_{irr}). Note that fast reactions equate to threshold reactions and thermal reactions are the non-threshold reactions.

Fast neutron fluences (for energies both greater than 0.1 MeV and greater than 1.0 MeV) are calculated using spectral-averaged cross sections that, ideally, should be average values from the neutron spectrum that represent the best estimate available. If an initial representation of the neutron flux spectrum is available (which is an input to STAYSL PNNL), then the user can perform a STAYSL PNNL FIR run (i.e., without spectral adjustment) to obtain cumulative integral flux values, from which spectral averaged cross sections can be determined. If the neutron spectrum is not known, then there are options (as discussed in Section 7.3) based on the U-235 fission spectrum or tables of evaluated nuclear data files.

Equation 35 shows the calculation of the fast neutron fluence, Φ_{fast}, based on the calculated sig-phi values (Equation 34), irradiation time, T_{irr}, and user specified cross sections, σ, for energies of "> 0.1 MeV" or "> 1.0 MeV." The constants in the equation are to convert time from days to seconds (i.e., 86400 $^{s}/_{day}$) and the cross section from barns to cm² (1E-24 barns/cm^2).

$$\Phi_{fast,i,j,k} = \frac{\sigma\phi_{i,j} \cdot T_{irr} \cdot 86400 \cdot 1\times10^{24}}{\sigma_{i,k}} \qquad \text{for the j}^{th}\text{ sample of the i}^{th}\text{ reaction and k = either "> 0.1 MeV" or "> 1.0 MeV"} \qquad (35)$$

Approximate thermal neutron fluences are calculated for non-threshold reactions from simplistic equations that use the cross sections for the target isotope in each reaction. Equation 36 shows the calculation of the uncorrected thermal neutron fluence, $\Phi_{thermal,\,uncorrected}$, which is the same formula as for Equation 35 except that the cross sections come from Table 2. The thermal neutron fluences provide a mechanism by which an estimate of the ratio of epithermal to thermal neutron fluences, $r_{epi:therm}$, can be optimized. The estimated $r_{epi:therm}$ is used with the thermal (2200 m/s) neutron cross sections and resonance integrals for the target isotopes (from Table 2) to calculate an epithermal correction factor, *ECF* (Equation 37). The *ECF* is, in turn, used to calculate an adjusted thermal neutron fluence, $\Phi_{thermal}$, with Equation 38. The epithermal/ thermal ratio, $r_{epi:therm}$, can be refined by minimizing the variance in the adjusted thermal neutron fluence between reactions for the same sample (or alternately, between all reactions for all samples).

$$\Phi_{thermal,uncorrected,i,j} = \frac{\sigma\phi_{i,j} \cdot T_{irr} \cdot 86400 \cdot 1\times10^{24}}{\sigma_{target,i}} \qquad \text{for the j}^{th}\text{ sample of the i}^{th}\text{ reaction} \qquad (36)$$

$$ECF_{i,j} = 1 + \left(\frac{RI_{target,i}}{\sigma_{target,i}}\right) \cdot r_{epi:therm,j} \qquad \text{for the j}^{th}\text{ sample of the i}^{th}\text{ reaction} \qquad (37)$$

$$\Phi_{thermal,i,j} = \frac{\Phi_{thermal,uncorrected,i,j}}{ECF_{i,j}} \qquad \text{for the j}^{th}\text{ sample of the i}^{th}\text{ reaction} \qquad (38)$$

It should be noted that these fast and thermal neutron fluence values, derived from simple approximations, are only provided for the purpose of checking data consistency and to give the user an initial estimate for those fluences.

The thermal neutron fluence values (Equation 38) form a basis for estimating the burn-up for fast (threshold) reactions. The average thermal neutron fluence is calculated, as shown in Equation 39, for each sample over all N_{rxn} thermal reactions (not including LI6A and B10A). As shown in Equation 40, this average thermal neutron fluence can then be converted to a flux (by dividing by the irradiation time) and then to a reaction-specific average thermal sig-phi value, $\sigma\phi_{avg\_thermal,\,i,\,j}$, that is applied in the burn-up calculations for fast reactions (Equation 31). If there are no thermal reactions being evaluated (neglecting LI6A and B10A), then the user must specify a value for $\Phi_{thermal,avg}$, which is used in Equation 40.

$$\Phi_{thermal,avg,\,j} = \frac{\sum_{i=1}^{N_{rxn}} \Phi_{thermal,i,\,j}}{N_{rxn}} \qquad \text{for the } j^{th} \text{ sample of the } i^{th} \text{ reaction} \qquad (39)$$

$$\sigma\phi_{avg\_thermal,\,i,\,j} = \frac{\Phi_{thermal,\,avg,\,j} \cdot rDenom}{T_{irr} \cdot 86400 \cdot 1 \times 10^{24}} \qquad \text{for the } j^{th} \text{ sample of the } i^{th} \text{ reaction} \qquad (40)$$

7.5.2 Assumptions/Limitations

The following assumptions were used in the development of the SigPhi Calculator software calculations.

- The "power," *P*, is entered in the same units as the FEE data used as input to the BCF code.
- Available material/reaction pairs are those defined in Table 2, which is contained on the Reaction_Data worksheet (Figure 21) of the SigPhi Calculator.
- The user either enters a reasonable estimate for the ratio of epithermal to thermal fluences or applies the optimization (with sufficient data to arrive at a solution).
- The user only enters data where indicated by the cell shading or font color.
- The neutron burn-up calculation in the user-defined function will converge within 1000 iterations at some tolerance equal to or greater than 3 significant digits.
- The neutron burn-up iterations may fail to converge (particularly for very high burn-up reactions) as a result of a calculational overflow. If the burn-up factor is less than 0.1, then a value of 0.1 is returned and highlighted to indicate that additional measures may be required to account for burn-up (or that the calculation cannot be performed for this scenario).
- The gamma self-shielding calculation for wire samples assumes that n=50 (i.e., 100 terms) will be sufficient to calculate the self-shielding.
- Neutron self-shielding is accounted for via the SHIELD code and not in the SigPhi Calculator.
- A manual estimate of the ratio of the epithermal to thermal fluences is assumed to be based on user expertise and relevant data.

The flux irradiation history correction factor must be accounted for by one of the three approaches discussed above: the BCF code or gamma-ray spectrum analysis software "Saturation Activity" or "Saturation Activity with Sampling Decay" correction types.

The ancillary fluence calculations are to be used for diagnostic purposes or rough estimates only; STAYSL PNNL must be applied to get values that are spectrally adjusted.

Unless the sample is a pure material, the user must provide a value for μ. Values of μ are provided for a select set of elements, but the software does not attempt to account for the potential combinations of elements in the material as impurities/alloys/compounds. Currently all samples must have the same μ and L for a given reaction.

In the case of thick (larger radius) wire samples, 100 terms of the summation calculations (Equation 27) may not be sufficient to fully account for gamma self-shielding.

To optimize the ratio of the epithermal to thermal fluences, there must be data for at least two thermal (non-threshold) reactions. Otherwise there is insufficient data with which to calculate variances that are used in the minimization search.

8.0 STAYSL PNNL

8.1 Introduction/Background/Purpose

As discussed in Section 1.2, STAYSL PNNL is a modern variant of the STAY'SL code [1, 2, 3, 4] developed by Dr. Perey at Oak Ridge National Laboratory (ORNL) in the late 1970s. The purpose of the STAYSL PNNL code is to solve the dosimetry neutron spectral adjustment problem using least-squares fitting methods. Neutron spectrum adjustment is performed to find a spectrum that, for specified dosimetry cross sections, will give the most likely fit to a set of measured activities (accounting for decay during the irradiation, neutron and gamma self-absorption, and burn-up).

Given a set of neutron activation rates measured in a nuclear fission reactor or at an accelerator-based neutron source, STAYSL PNNL uses a generalized least-squares approach to determine the neutron flux spectrum. This process is referred to as neutron spectral adjustment [13, 14, 15], since the preferred approach is to use measured data to adjust neutron spectra provided by reactor physics calculations. Application of STAYSL PNNL uses the corrected activation rates calculated in the SigPhi Calculator, the neutron self-shielding correction factors (from SHIELD), the cross section and covariance data libraries (from NJOY99/NJpp), along with the initial estimate of the neutron flux spectrum (preferably from reactor physics calculations, such those performed by the MCNP code [16, 17]). The output of a STAYSL PNNL application run provides the adjusted neutron spectrum and a brief summary of broader group fluxes and the covariance matrix. Reaction rates and spectral-averaged activation cross sections are also calculated for the convenience of the user for all of the reactions in the nuclear data library. The output can subsequently be used for reactor dosimetry or radiation damage assessments.

STAYSL PNNL is used in conjunction with the other software in the STAYSL PNNL suite to analyze monitor sample data that is specific to the neutron flux and sample material/geometry used in a particular irradiation event.

8.2 Installation, Uninstallation, and Updating

STAYSL PNNL is a command line program that does not require any particular installation/un-installation procedures per se on a Windows-based personal computer. The STAYSL PNNL code comes as a compiled executable file "staysl_pnnl.exe" that the user can simply place in any convenient directory. However, to execute the STAYSL PNNL code, the executable must be either located in the active directory from which it is being executed or it must be found in a directory in the command line window's search path. Section 3.2 describes the approaches to starting a command line program and how to modify the system search path (substitute STAYSL PNNL-specific information for path and executable, i.e., "staysl_pnnl.exe").

STAYSL PNNL can be uninstalled simply by deleting the "staysl_pnnl.exe" file and/or the associated program directory (e.g., "C:\Apps\STAYSL_PNNL\"). If the user altered the standard search path, then the user should manually undo that change.

STAYSL PNNL is updated simply by replacing the "staysl_pnnl.exe" file with a new file. The STAYSL PNNL version number and date are displayed when the code is run.

See also Section 1.5 for information on automated installation and updates to the PATH environment variable.

8.3 Input Data and Run Options

The STAYSL PNNL code requires four ASCII text input files: a cross sections data library, a cross section covariances data library, a neutron self-shielding data library, and a run parameters input file. The content of these former two libraries, derived from IRDF-2002 data (Section 2.2) that is extracted and formatted via the NJOY99 (Section 3.0) and NJpp (Section 4.0) codes, is specified (based on Table 2) and would only change via the formal software change request process. The neutron self-shielding data library is generated via the SHIELD code (Section 5.0) and may apply to more than one STAYSL PNNL analysis, depending on the nature of the monitor samples. The formats of the data libraries are described in Sections 4.4 and 5.4. The data library files must be named "xsectlib.dat," "covarlib.dat," and "sshldlib.dat," for the cross sections, covariances, and neutron self-shielding, respectively.

The run parameters input file contains the data and options that define the application run scenario for STAYSL PNNL. The run parameters file name can be supplied as a command line argument when executing "staysl_pnnl.exe," or will be requested via an interactive prompt, and can be any convenient name. Each run parameters input file will contain information specific to a particular irradiation and a particular monitor sample, although multiple reactions can be analyzed for that sample (indeed, multiple reactions are required for a meaningful least-squares solution). Other samples would be analyzed in separate application runs. The STAYSL PNNL run parameters input file is generated manually based on details of a specific scenario, although some of the run parameters input file information comes directly from the SigPhi Calculator results (see Section 7.4). The user must ensure that the run parameters input file data (units, etc.) is consistent with information used in the other STAYSL PNNL suite software for analysis of a particular irradiation scenario. Table 7 describes the structure of the run parameters input file and the meaning of the parameters, including valid options. Note that when data are required in the form of a lower triangular portion of a symmetric matrix, the diagonal and all off diagonal values below/to the left of the diagonal must be supplied in the conventional row by row order.

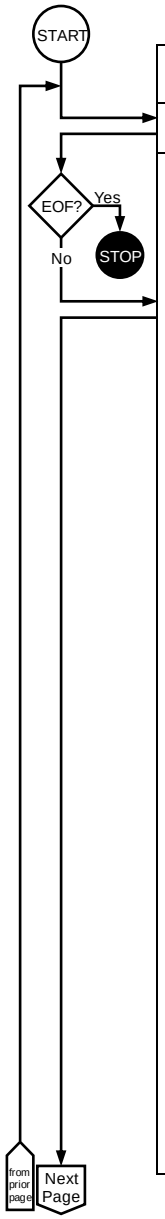
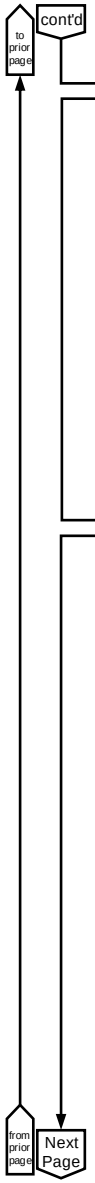


Table 7. *Structure of the run parameters input data file for the STAYSL PNNL code.*

Record #	When Required	# Repetitions of the Record	Variables (Dimensions)	Fortran Format	Description of Variables & Valid Values
1	Always	No repetition	sTITLE	A80	Title text for the STAYSL PNNL run
2	Always	No repetition	KG, KA, IPNT, IACT, KQT	5I5	KG – Number of energy grid groups (i.e., one less than the number of energy grid group boundaries) KA – Number of reactions (each with a reaction rate from SigPhi Calculator) IPNT – Flag to define certain output options This flag serves to modify the output to the "<stayslin>.out" and "sta_spe.dat" files. So-called "normal" output to the "<stayslin>.out" file may be supplemented or constrained based on IPNT. The "sta_spe.dat" file is not generated unless specified by this flag. See Section 8.4 for a detailed description of the STAYSL PNNL output. See also the description of the Record 5 A0 parameter. 0 Provide normal output, plus the following additional information: the dosimetry data input correlation matrix, the relative covariance matrix of activities, the contribution due to input flux covariance matrix, the contribution due to input cross section covariance matrix, the input dosimetry cross sections, a table of the energy group-specific adjusted differential flux and associated standard deviation, and the full input flux correlation matrix. 1 Provide normal output only 2 Provide normal output, but suppress output of the input/output flux correlation matrices 3 Provide normal output and generate the "sta_spe.dat" file to contain the energy dependent (i.e., group by group) adjusted reaction rates 4 Provide normal output and generate the "sta_spe.dat" file to contain energy dependent (i.e., group by group) cover corrections to the reaction rates IACT – Flag to define spectral adjustment options Note that the program always (except for the FIR run described for Record 5 parameter A0) gives a summary of reaction rates for all reactions at the end of the primary output file. 0 Perform spectral adjustment 1 Perform an "activity run" (calculating reaction rates) without any spectral adjustment calculations, computing reaction rates for the provided spectrum KQT – Flag to define the group-by-group flux input type (affects Record 19) 0 Differential Flux 1 Group Flux (i.e., Differential Flux × ΔE) 2 Differential Flux × $E_{average}$

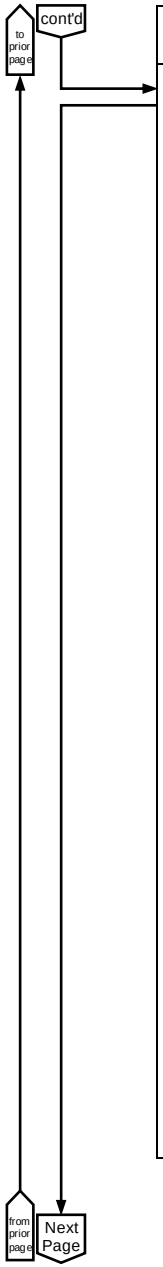
Note: EOF = End of file; the EOF decision shown above is a byproduct of trying to read the next record 1 entry with failure to read due to EOF telling the code that the run is done

***Table 7**. Continued.*



Record #	When Required	# Repetitions of the Record	Variables (Dimensions)	Fortran Format	Description of Variables & Valid Values
3	Always	No repetition	`ACVX, FCHN, FCVX, FS`	`free (R,R,R,R)`	ACVX – Flag and a value pertaining to cross-correlations between the different activities < 0 Read activity covariance data as the lower triangular portion of a full KA × KA matrix (assumed symmetric, but enter lower portion only) ≥ 0 Set the off-diagonal activity covariance matrix values to (ACVX)² FCHN – Flag and a value pertaining to flux covariances ≤ 0 Read in and expand the group flux covariance matrix > 0 Use Gaussian formalism to define the flux covariance matrix; this value is full width at half max. of short range Gaussian covariance for flux FCVX – Value of the long-range covariance for flux This value is required regardless of the value of FCHN. Value is used in a Gaussian calculation, so should typically be a positive value. FS – Value of cross-correlation between cross sections of different reactions
4	Always	No repetition	`AK1, NORML, ILOG, TIME, ACNM`	`free (R,I,I,R,R)`	AK1 – Flag (non-negative value) pertaining to normalization of the input flux This value is scaled by the ACNM renormalization factor. = 0.0 Automated normalization of input flux is performed prior to spectral adjustment; back AK1 out of RENORM by dividing out ACNM 1.0 No normalization is performed (aside from ACNM renormalization) > 0 The value provided (≠ 1.0) is used as the normalization factor; use for small adjustments; use TNORM (record 16) for large adjustments NORML – Flag to define how to perform flux normalization when AK1 = 0 ≠ 1 Flux normalization by chi-square (preferred approach) 1 Flux normalization by standard deviation ILOG – Flag to define whether to use logarithmic or linear approaches for flux adjustment ≤ 0 Apply logarithmic adjustments when needed to avoid negative fluxes > 0 Always apply linear adjustments, even if that results in negative fluxes TIME – Length of the irradiation duration, in seconds This value may represent the total actual time or the effective full power time and will typically be consistent with the SigPhi Calculator. This value is merely used to compute collapsed grid fluence values for user convenience. ACNM – Renormalization factor to adjust between types of time If the TIME value is consistent with the SigPhi Calculator, then ACNM should be set to 1.0. If TIME represents actual time and effective full power time was used in the SigPhi Calculator, then ACNM should be set to 1/RNF (Section 7.3). If TIME represents effective full power time and actual time was used in the SigPhi Calculator, then ACNM should be set to the quotient of the full power divided by the AVGBM.

***Table 7**. Continued.*



Record #	When Required	# Repetitions of the Record	Variables (Dimensions)	Fortran Format	Description of Variables & Valid Values
5	Always	KA	sIREA (KA), A0 (KA), SDA (KA), sIDM (KA), CD (KA), sIRSH2 (KA), FSHLD (KA), sFLDV (KA)	A8, E10.3, F6.3, 1X, A4, F6.2, 1X, A4, F6.2, 1X, A3	sIREA – Short name of reaction A0 – Reaction rate (activity) for the reaction (atom/atom-s) For a future irradiation run (FIR), which simply calculates the reaction rates for the user-specified reactions without adjusting the neutron flux spectrum, leave this value blank or set to 0.0 for the first record 5 entry (other record 5 A0 values are ignored if the first one is blank or 0.0). SDA – Uncertainty in the reaction rate sIDM – Four-character identifier for the cover associated with the reaction If no cover and no self-shielding apply, then this value and the rest of the record may be left blank. If self-shielding applies, but no cover was used, then use spaces as placeholders for this value. 'BORO' Boron cover 'CADM' Cadmium cover 'GADO' Gadolinium cover 'GOLD' Gold cover CD – Flag and the value of the cover thickness Value stated in mils (thousandths of an inch). If no cover was used, then set this value to zero. If this value is missing or negative, then a value of 0.0 is applied. ≤ 0.0 Do not account for cover effects > 0.0 Apply this dimension in the cover calculations sIRSH2 – Four-character, user-selected device (sample) variant code Value must match the corresponding entry in the 'sshldlib.dat' file. If self-shielding is not calculated, this parameter may be absent. FSHLD – Flag and the value of the mean chord of wire or thickness of foil Value stated in mils. If this value is missing or negative, then a value of 0.0 is applied. ≤ 0.0 Do not account for self-shielding effects > 0.0 Apply this dimension in the self-shielding calculations sFLDV – Code for the type of flux applied and the type of device (sample) This value is not required if there is no cover and no self-shielding. If self-shielding is applied, this value must be consistent with the corresponding entry in the 'sshldlib.dat' file. 'BFX' Beam flux, Foil device 'IFX' Isotropic flux, Foil device 'BWX' Beam flux, Wire device 'IWX' Isotropic flux, Wire device

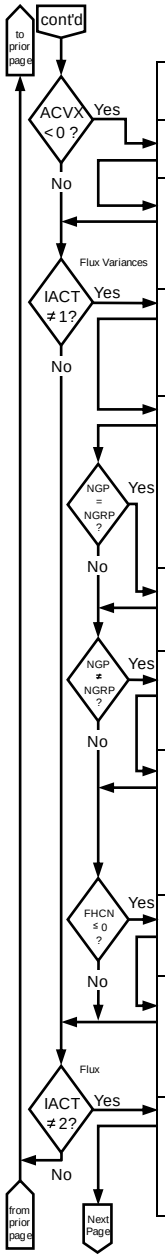
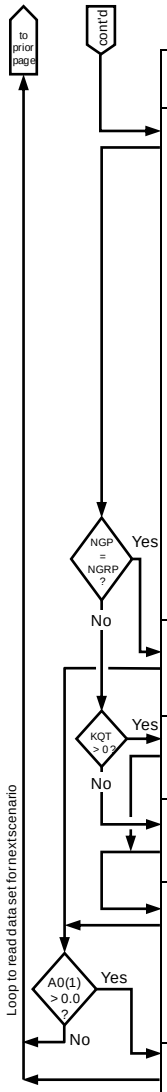


***Table 7**. Continued.*

Record #	When Required	# Repetitions of the Record	Variables (Dimensions)	Fortran Format	Description of Variables & Valid Values
6	ACVX < 0	No repetition	`sDUM`	`A80`	Annotation describing the activity covariance data
7	ACVX < 0	No repetition (but the array is read in an implied DO loop)	`siIC (KA,KA)`	`free (I)`	Activity covariance data Provide this data as the lower triangular portion of a full symmetric KA × KA matrix (supplying an upper triangular matrix isn't equivalent).
8	IACT ≠ 1 (applies to records 8-15 as a group, but is explicitly stated for each)	No repetition	`sSPECT`	`A80`	Annotation describing the subsequent group flux uncertainty data Note: records 8-14 are read via the GetFluxVar() subroutine.
9	IACT ≠ 1	No repetition	`NGP`	`I4`	NGP – Number of energy grid groups (i.e., one less than the number of energy grid group boundaries) If this number doesn't equal the number of groups for the energy grid in the cross section data file (NGRP), then the flux uncertainty will be interpolated to the energy grid from the cross section data file.
10	IACT ≠ 1 and NGP = NGRP	No repetition (but the array is read in an implied DO loop)	`FERR (NGRP)`	`free (R)`	Flux uncertainty data (aligned energy grid) (NGRP = number of energy grid groups in the cross section data file)
11	IACT ≠ 1 and NGP ≠ NGRP	No repetition (but the array is read in an implied DO loop)	`EIN (NGP+1)`	`free (R)`	Energy grid groups for flux uncertainty Read NGP values (although the array is dimensioned one element larger).
12	IACT ≠ 1 and NGP ≠ NGRP	No repetition (but the array is read in an implied DO loop)	`FUIN (NGP+1)`	`free (R)`	Flux uncertainty data (non-aligned energy grid) Read NGP values (although the array is dimensioned one element larger). These values are interpolated to FERR (which uses the standard 100-group energy grid). Linear interpolation is used when FUIN is less than 1.0E-36 and log-log interpolation otherwise.
13	IACT ≠ 1 and FCHN ≤ 0	No repetition	`sDUM`	`A80`	Annotation describing the subsequent flux group covariance data
14	IACT ≠ 1 and FCHN ≤ 0	No repetition (but the array is read in an implied DO loop)	`JF (NGP,NGP)`	`free (I)`	Flux group covariance data Provide this data as the lower triangular portion of a full symmetric NGP × NGP matrix (supply lower portion only). Values must be integers that have been scaled by a factor of 1000 (i.e., 1.0 → 1000).
15	IACT ≠ 2 (applies to records 16-21 as a group, but is explicitly stated for each)	No repetition	`sSPECT`	`A80`	Annotation describing the subsequent flux data Note: records 15-19 are read via the GetFluxVar() subroutine

***Table 7**. Continued.*



Record #	When Required	# Repetitions of the Record	Variables (Dimensions)	Fortran Format	Description of Variables & Valid Values
16	IACT ≠ 2	No repetition	`NGP, ITHERM, TNORM, TMPR, ETE`	`I4, I4, F10.4, F10.4, F10.4`	NGP – Number of energy grid groups (i.e., one less than the number of energy grid group boundaries) If this number doesn't equal the number of groups for the energy grid in the cross section data file (NGRP), then the flux will be interpolated to the cross section data file energy grid. ITHERM – Flag indicating whether to add a thermal Maxwellian below a given neutron energy ≤ 0 Do not add a thermal Maxwellian > 0 Add a thermal Maxwellian TNORM – Multiplicative normalization factor applied to the flux If this value is less than or equal to zero (or missing), then a value of 1.0 is applied. TMPR – Temperature of the thermal Maxwellian (°C) If this value is zero (or missing), then a value of 20.0 °C is applied. ETE – Inverse joining energy (i.e., 1/E, in MeV) A thermal Maxwellian is applied for energies below this value, when ITHERM > 0. If this value is zero (or missing), then a value of 5.0E-8 MeV is applied.
17	IACT ≠ 2 and NGP = NGRP	No repetition (but the array is read in an implied DO loop)	`F (NGRP)`	`free (R)`	Flux spectrum data (aligned energy grid) The data type is determined by the KQT parameter. (NGRP = number of energy grid groups in the cross section data file)
18a	IACT ≠ 2 and NGP ≠ NGRP and KQT > 0	No repetition (but the array is read in an implied DO loop)	`EIN (NGP+1)`	`free (R)`	Energy grid group boundaries for flux data Read NGP+1 values.
18b	IACT ≠ 2 and NGP ≠ NGRP and KQT ≤ 0	No repetition (but the array is read in an implied DO loop)	`EIN (NGP+1)`	`free (R)`	Midpoint energy for each of the energy grid groups for the flux data Read NGP values (although array is dimensioned 1 element larger).
19	IACT ≠ 2 and NGP ≠ NGRP	No repetition (but the array is read in an implied DO loop)	`FIN (NGP+1)`	`free (R)`	Flux spectrum data (non-aligned energy grid) Read NGP values (although the array is dimensioned 1 element larger). These values are interpolated to F (based on the standard 100-group energy grid). Linear interpolation is used when FIN is less than 1.0E-36 and log-log interpolation otherwise. The data type is determined by the KQT parameter.
20	IACT ≠ 2 and A0(1) > 0.0	No repetition (but the array is read in an implied DO loop)	`clN (10)`	`free (I)`	Number of groups spanned for each bin of a ten-element mini-spectrum Number of the full energy grid groups (out of NGRP) to collapse into each bin of a 10-group mini spectrum, starting from the lower energies in the first bin. The mini-spectrum grid is for ease of reporting or viewing fluxes and covariances and has no effect on the adjustments calculated by the program.

Although not recommended (as noted in Section 7.4), it is possible for advanced users to alter the time basis in STAYSL PNNL from that used in the SigPhi Calculator. That is, the user can change from an effective full power time used in the SigPhi Calculator to actual irradiation time (or vice versa). Changing the time basis requires that the user manually change the values for both the TIME and the ACNM input parameters. The description of record 4 in Table 7 discusses how the values must be changed. When ACNM is not unity, the normalization applied via the AK1 parameter is automatically adjusted to maintain the correct normalization of the input spectrum. Thus, no modification of AK1 is required when implementing a manual change (via TIME and ACNM) in time basis (from effective to actual or vice versa). Note that concurrently applying automated normalization of the input flux (AK1 = 0.0) and a change in time basis (ACNM ≠ 1.0), does not particularly make sense, but is allowed. In such a case, the user could divide the RENORM value in the primary output file by ACNM to obtain the effective value of AK1.

The user can easily determine if the change to the time basis was done correctly in STAYSL PNNL because the calculated neutron fluence values in the output file should always be the same, regardless of the ACNM normalization. However, the neutron flux values will change when the time basis changes. The discussion around Figure 7 in Section 1.3.2 explains this relationship between time, flux, and fluence. Table 8 lists the settings required for all four permutations of effective time and actual irradiation time to produce the same fluence. In general the AK1 value does not need to be changed for a change in time basis, but AK1 is modified here to give the same fluence results.

Table 8. *Manual adjustment of key STAYSL PNNL input parameters related to a change in time basis such that each configuration gives the same fluence results.*

		STAYSL PNNL Input [a]	
		Effective Full Power Time	Actual Irradiation Time (including outages)
Sig-Phi Calc. Output	Effective Full Power Time	$A0 = A0_E$ $TIME = TIME_E$ $ACNM = 1.0$ $AK1 = AK1_E$	$A0 = A0_E$ $TIME = TIME_A$ $ACNM = 1.0 / RNF$ $AK1 = AK1_E$
	Actual Irradiation Time (including outages)	$A0 = A0_A$ $TIME = TIME_E$ $ACNM = RNF$ $AK1 = AK1_E / RNF$	$A0 = A0_A$ $TIME = TIME_A$ $ACNM = 1.0$ $AK1 = AK1_E / RNF$

[a] Information unchanged from the Sig-Phi Calculator is shown in Blue; information manually set/changed in the STAYSL PNNL run parameters input file is shown in Green. Subscript "E" denotes effective full power time, while subscript "A" denotes actual irradiation time (including periods of zero power). A0 refers to the sig-phi values (activities; reaction rates). TIME, ACNM, and AK1 are input parameters (record 4 of Table 7). RNF is the renormalization factor calculated in the Sig-Phi Calculator when using effective full power time (see also Equation 20). The only reason to change AK1 would be to obtain the same fluence for all four scenarios shown; if just changing the time basis, no change to AK1 is required (i.e., each row has the same AK1 value for both scenarios).

This approach of manually changing the time basis adds unnecessary complexity that is best to simply avoid by (re-)running the desired time scenario in the SigPhi Calculator.

Three modes of operation for STAYSL PNNL are indirectly noted in the Table 7 descriptions of input file records 2 and 5. Most often, STAYSL PNNL will be run in the standard mode where reaction rates (sig-phi values) and a neutron flux spectrum are entered, resulting in adjusted outputs. However, there are times when unadjusted information is useful in evaluating future experiments or in specific calculations. An "activity run" can be performed by setting IACT equal to a value of 1 (in record 2). No input reactions/activities (i.e., record 5 entries) are required for an "activity run"—that is, KA can be set to zero. Any reactions/activities specified in an "activity run" are ignored. The activity run produces a table of reaction rates (sig-phi) and cross sections (sig) for all reactions in the cross section library based on the input flux spectrum. The FIR run mode is intended to provide information useful for assessment of "future irradiation experiments." The FIR run mode is specified by setting the activity for the first record 5 entry of reactions to a value of 0.0 or by leaving the activity blank. In FIR mode, the activities of other record 5 entries are ignored. Note that a FIR run cannot be signaled by zero or blank activity data in any record 5 entry other than the first one. The FIR run will produce a list of unadjusted reaction rates (sig-phi) and cross sections (sig) for the reactions specified with a record 5 entry. Although unadjusted, these values will include corrections for any specified covers or self-shielding. A FIR run also produces a table in which the differential flux spectrum and the integral (cumulative) flux for the portion of the spectrum greater than the noted energy are listed. Table 9 summarizes the distinguishing features between the STAYSL PNNL run modes.

Table 9. *Features of the normal, FIR run, and activity run modes for STAYSL PNNL.*

Mode	Flag to Indicate Mode	Activities/ Cross Sections Account for self-shielding?	Activities/ Cross Sections Account for Covers?	Use AK1 [a] and ACNM?	Reactions Reported	Information in the Primary Output File
Normal Run	IACT = 0 A0(1) > 0.0	Yes	Yes	Yes	Reactions requested in Record 5 entries and all reactions in the cross section library	Table of activities for specified reactions before and after flux spectrum adjustment. Table of group-by-group differential flux and integral flux > specified energy. Table of adjusted reaction rates (activities, Sig-Phi) and cross sections (Sig) for all library reactions.
Activity Run	IACT = 1 A0 ignored (if present)	No	No	No	All reactions in the cross section library	Unadjusted reaction rates (activities, Sig-Phi) and cross sections (Sig)
FIR Run	IACT = 0 A0(1) = 0.0	Yes	Yes	No	Only reactions requested in Record 5 entries	Unadjusted reaction rates (activities, Sig-Phi) and cross sections (Sig). Table of group-by-group differential flux and integral flux > specified energy.

[a] AK1 is the flux normalization factor (user specified or automatically calculated). ACNM is a renormalization factor pertaining to the time basis for the input activities and will normally be 1.0 unless manually altered as described earlier in this section.

8.4 Output

There are five potential structured ASCII text output files generated by STAYSL PNNL. The "<stayslin>.out" (OUT) file (where <stayslin> is the input file name without any file extension) is the primary output file, which is always created. Two additional output files that are created

with each STAYSL PNNL standard (normal) application run are the "sta_xfr.dat" and "sta_dam.dat" files, with the former file containing spreadsheet-importable data (which contains a three-column listing of the energy, unadjusted neutron flux, and adjusted neutron flux spectrum for plotting applications) and the latter file comprising an input file for use with SPECTER (see Section 9.0). If an activity run is being performed, the "sta_xfr.dat" and "sta_dam.dat" files are not produced because the objective is to simply output the unadjusted reaction rates and cross sections for all library reactions. If the input run parameters indicate that an FIR run is being performed, then the "sta_fir.dat" file is created (instead of the "sta_xfr.dat" and "sta_dam.dat" files) to receive output data useful for scoping calculations to determine how much material should be irradiated in a future experiment. If the IPNT input parameter (in record 2, as shown in Table 7) is set to a value of 3 or 4, then the energy dependent (i.e., group-by-group) reaction rates or cover corrections to the reaction rates, respectively, are output to the fifth potential output file titled "sta_spe.dat," (regardless of the normal/FIR/activity run mode). Note that if none of the specified reactions in the input file have a cover when IPNT=4, then the "sta_spe.dat" file is not produced because there is no information to output.

In all STAYSL PNNL run modes (normal, activity run, FIR run), the primary output file consists of two sections. The first section contains an echo of all the input run parameter values that were read and validated by the STAYSL PNNL code. This first section is reproduced for two potential uses: to confirm that the inputs used in the run are the expected values and/or to supply the formatted input for another STAYSL PNNL application run (i.e., if the original input is not available). The end user is encouraged to do a file comparison on the run parameters input file and the primary output file to detect errors in specifying the input. The second section of the primary output file contains self-documenting output from the calculations performed in STAYSL PNNL. The content of this second portion depends on the operational mode of the run and the print output option (IPNT) selected. A standard run will include multiple blocks/tables of output, with appropriate headings to identify the nature of the data. The blocks of data for all modes and print options are described in Figure 29 and an example of extended output (IPNT = 0) for a normal STAYSL PNNL run is provided in Appendix B. The output in this second section should be examined for any potential issues (very large/small numbers, "NaN," "Infinity," warning messages, etc.) that may indicate input errors or incorrect input data.

The main output from a STAYSL PNNL activity run (Table 9) is a table of unadjusted reaction rates (sig-phi) and cross sections (sig) for all reactions in the cross section library. These values are based on the input flux spectrum, accounting for temperature normalization (TNORM), but not for covers, self-shielding, or flux normalization (AK1).

A STAYSL PNNL FIR run will produce a list of unadjusted reaction rates (sig-phi) and cross sections (sig) for only the reactions specified with a record 5 entry in the run parameters input file (Table 7). These values include corrections for any specified covers or self-shielding and any temperature normalization (but not flux normalization). A FIR run also produces a table listing the unadjusted differential flux spectrum and the integral (cumulative) flux (i.e., for the portion of the spectrum greater than the noted energy).

Echo of run parameters input file (i.e., reflecting data/options per Table 7)	All run modes
Output heading, denoting the version of STAYSL PNNL	All run modes
Scenario heading, denoting the title annotation, number of energy groups, number of reactions, and ACNM	All run modes
Covariance parameters block (FCHN, FCVX, ACVX, FS, value of the determinant, and error)	Normal run, all IPNT
Input normalization parameters (AK1, VAK, NORML, AK·ACNM, CHI², Normalized CHI²)	Normal run, all IPNT
Table of Dosimetry Activities (inputs, unadjusted, adjusted, Chi², energy range for 90% of the activity, and standard deviations)	Normal run, all IPNT
Dosimetry Data Input Relative Correlation Matrix	Normal run, IPNT = 0 only
Relative Covariance Matrix of Activities	Normal run, IPNT = 0 only
Contribution due to Input Flux Covariance Matrix	Normal run, IPNT = 0 only
Contribution due to Input Cross Section Covariance Matrix	Normal run, IPNT = 0 only
Input Dosimetry Cross Sections (group by group, unadjusted cross sections, includes cover, self-shielding, and normalization corrections)	Normal run, IPNT = 0 only
Differential Fluxes (group-by-group, unadjusted and adjusted, differential flux and standard deviations, integral flux)	Normal run, all IPNT
Integrals of Spectra	Normal run, all IPNT
New Differential Fluxes (group-by-group adjusted fluxes and standard deviations)	Normal run, IPNT = 0 only
Summary of Broad-Group Fluxes, Fluences, And Uncertainties (irradiation time, flux/fluence for specific energy regions [epithermal, thermal, and fast], flux/fluence for the Mini-Spectrum, relative covariances for Mini-Spectrum)	Normal run, all IPNT
Spectral-Averaged Reaction Rates (sig-phi and sig for all cross section library reactions)	Normal run, all IPNT
Input Flux Relative Correlation Matrix (by row from diagonal, 100×100 matrix)	Normal run, 1st row only in IPNT = 1, not in IPNT = 2
Output Flux Relative Correlation Matrix (by row from diagonal, 100×100 matrix)	Normal run, not in IPNT = 2
Unadjusted Reaction Rates (sig-phi and sig for all cross section library reactions)	Activity run only
Calculated Activities (unadjusted sig-phi and sig, including any cover or self-shielding factors)	FIR run only
Spectrum for Activities (group-by-group unadjusted differential flux and integral flux > E)	FIR run only

Figure 29. *Overview of the structure of the primary output file (left pane) from a STAYSL PNNL run. Elements specific to IPNT or run mode options are denoted in the right pane.*

A FIR run will also produce an ancillary file titled "sta_fir.dat," which contains a list of the reactions and their unadjusted reaction rates, accounting for any specified covers or self-shielding and for any temperature normalization (but not flux normalization). This file includes the same information as available in the primary output file, but can be used as input to other calculational tools (e.g., the SCOPER code [unpublished]). The structure of the "sta_fir.dat" file is depicted in Figure 30.

Record 1: <Number of reactions, KA> 1.0000E+00
Record 2: <Short reaction name> <Reaction rate, unadjusted, accounting for any cover or self-shielding, ES10.4 format>
— Repeat record 2 for each reaction —

Figure 30. *Structure of the STAYSL PNNL "sta_fir.dat" output file. The second number of the first record represents the flux normalization, which is always set to 1.0 for a FIR run.*

The "sta_xfr.dat" file, produced in the normal run mode of STAYSL PNNL, contains a three-column listing of the neutron flux spectrum data that is suitable for importing into spreadsheet or plotting applications. Figure 31 describes the structure of the "sta_xfr.dat" file. Group-by-group data for the differential flux times the average group energy is provided for creating a step plot. Note that the energy grid used (as with nearly everything in STAYSL PNNL) is that specified in the cross section library. Both unadjusted and adjusted neutron flux are included in the output. The unadjusted flux includes any temperature normalization (TNORM) and flux normalization (AK1), thus may differ from the input flux spectrum by a constant.

Record 1: "E (MeV)"<tab>"Unadj. F×Eavg"<tab>"Adj. F×Eavg"
Record 2: <Energy boundary, ES12.5 format><tab><Unadjusted differential flux times average group energy, ES12.5 format><tab><Adjusted differential flux times average group energy, ES12.5 format>
Record 3: <Next higher energy boundary, ES12.5 format><tab><Same unadjusted differential flux times average group energy as in Record 2, ES12.5 format><tab><Same adjusted differential flux times average group energy as in Record 2, ES12.5 format>
— Repeat records 2 & 3 for each energy group —

Figure 31. *Structure of the STAYSL PNNL "sta_xfr.dat" output file, giving differential flux times average group energy in a format suitable for plotting.*

The "sta_dam.dat" file, produced in the normal run mode of STAYSL PNNL, contains data that feeds directly into the SPECTER code (see Section 9.0) for radiation damage calculations. Thus the structure of the "sta_dam.dat" file (Figure 32) is dictated by the SPECTER code. The file contents consist of the energy grid, the adjusted neutron flux spectrum, and the associated flux covariances.

Record 1: <sTitle from Record 1 of the STAYSL PNNL run parameters input file>
Record 2: 2 0 0 1 <ACNM, in ES11.4 format><TIME, in ES11.4 format>
Record 3: <Number of energy groups, M, in I5 format> 1
Record 4: <Array of energy structure boundary values, 8 columns wide, in ES10.3 format, wrapping to the next line>
Record 5: <Array of adjusted differential flux values, 8 columns wide, in ES10.3 format, wrapping to the next line>
Record 6: <Flux covariance terms, written as M blocks of data, each up to 8 columns wide, in ES10.3 format, and wrapping to the next line>

Figure 32. *Structure of the STAYSL PNNL "sta_dam.dat" output file. Note that the numbers in records 2 and 3 are unchanging constants (in I2 and I5 format, respectively).*

When the STAYSL PNNL input parameter IPNT (record 2 in Table 7) is specified as a value of 3 or 4 the "sta_spe.dat" file is produced, with the contents depending on the IPNT value. For IPNT = 3, the "sta_spe.dat" file (Figure 33) contains the energy dependent (i.e., group-by-group), adjusted reaction rates, accounting for any specified covers, self-shielding, and normalization. For IPNT = 4, the "sta_spe.dat" file (Figure 34) contains the energy dependent cover correction factors and component values (density, cover thickness, cover cross section, and the exponential term [see Equation 41]).

Record 1: <header line with “Energy (MeV)” and reaction long names as tab-delimited values>
Record 2: <Energy grid boundary value, in ES12.5 format><tab><adjusted reaction rate for 1st reaction, in ES12.5 format><tab><adjusted reaction rate for 2nd reaction, in ES12.5 format> and so on for all reactions…
— Repeat record 2 for each energy group in the cross section library energy grid —
Record 3: <Uppermost energy grid boundary value, in ES12.5 format>
Record 4: <trailing blank line>

Figure 33. *Structure of the STAYSL PNNL “sta_spe.dat” output file when the IPNT input parameter is set to a value of 3, giving the adjusted reaction rates.*

Record 1: “Reaction: ”<tab><Reaction long name><tab>“Flux Type: ”<tab><Flux type code>
Record 2: “Cover: ”<tab><Cover name><tab>“Cover Thickness: ”<tab><Cover thickness value (mil), ES12.5 format>
Record 3: “Cover Density: ”<tab><Cover material density value (g/cm³), ES12.5 format><tab>“Cover At. Wt.: ”<tab><Cover material atomic weight, ES12.5 format>
Record 4: “Energy (MeV)”<tab>“CCF”<tab>“SS”<tab>“Cover SIG”
Record 5: <Energy grid boundary value, in ES12.5 format><tab><cover correction factor, in ES12.5 format><tab><exponential term, in ES12.5 format><tab><cover cross section (barns), in ES12.5 format>
— Repeat record 5 for each energy group in the cross section library energy grid —
Record 6: <Uppermost energy grid boundary value, in ES12.5 format>
Record 7: <trailing blank line>
— Repeat records 1-7 for each reaction that has a cover specified —

Figure 34. *Structure of the STAYSL PNNL “sta_spe.dat” output file when the IPNT input parameter is set to a value of 4, giving cover correction factors and related quantities.*

8.5 Calculations

The primary calculations performed by STAYSL PNNL for spectral adjustment are described in the report for the STAY’SL code by Perey [1], to which the reader is referred for details. These calculations can be summarized by the following steps.

- Collect the input data for the saturated activities (of a set of user-specified reactions), the assumed flux spectrum, the reaction cross sections, and the associated covariances for these data.
- Calculate the activity covariance matrix (NAo)
- Calculate the C-matrix based on the flux spectrum and the cross sections.
- Calculate U-matrix from the flux covariance and the C-matrix.
- Calculate the A-vector as the sum of rows of the C-matrix.
- Calculate the flux covariance matrix (NAp) based on the C- and U-matrices.
- Calculate the cross section covariance matrix (NAs).
- Sum the covariance matrices (NAo + NAp + NAs) and invert the summed matrix to get the W-matrix.
- Minimize the chi-squared values based on the activities and the W-matrix.
- Calculate the output flux spectrum and associated relative covariance based on the minimized chi-square solution.

STAYSL PNNL uses least-squares fitting to perform neutron spectral adjustment instead of solving the “dosimetry unfolding problem” by iterative modification of an initial spectrum.

Older computer codes, such as SANDII [82], used an iterative process to determine a neutron spectrum that fit all the data. However, this approach does not take into account the full variance-covariance matrix and thus does not ensure that the best fit to the data will be found. Additionally, iteration methods provide little or no information about the uncertainty of the solution. Current practice is to refer to the process as an adjustment rather than "unfolding," since the starting neutron spectrum should be a physics-based calculation (such as from MCNP [16, 17] or other computer codes). Ideally, the starting point would include an estimate of uncertainties and covariances, to the extent that such information is available, for the activation data, dosimetry cross sections, and input group neutron fluxes (all assumed to have independent probability density functions). The least-squares spectrum adjustment method used by STAYSL PNNL takes into account all such available information. The spectrum adjustment solution procedure is fast (requiring only the inversion of a small matrix having dimensions equal to the number of activation measurements) and results in a statement of the uncertainties in the group fluxes due to the uncertainties in the input data. The matrix to be inverted will very seldom be singular; therefore, a solution may almost always be obtained. The solution obtained with the least-squares spectrum adjustment method is the best possible one in the sense that the uncertainty (covariance) of the solution is minimized.

8.5.1 Self Shielding and Cover Correction Factors

A separate computer code (SHIELD) is used to calculate neutron self-shielding corrections based on device geometry. The data for self-shielding corrections is read in through the "sshldlib.dat" data library and applied per the options selected in Record 5 of the input (Table 7).

A cover correction factor, *CCF*, is calculated based on the material, the atom density, the cover thickness, and the cross section, as shown in Equations 41 and 42. Here N_A is Avogadro's constant (equal to 6.02214129×10^{23} atom/mol [57]), ρ is the density of pure cover material (g/cm³), σ is the thermal neutron absorption cross section (barn), L is the cover thickness (mil), and MW is the atomic mass of the cover material (g/mol). The density and atomic mass data shown in Table 10 are included internally in STAYSL PNNL for use in this calculation based on the user-specified cover material. Cross section values are retrieved from the STAYSL PNNL cross section library.

$$SS = \frac{N_A \cdot \rho \cdot \sigma \cdot L}{MW} \cdot \frac{10^{-24} cm^2}{barn} \cdot \frac{2.54\times10^{-3} cm}{mil} \tag{41}$$

$$\begin{aligned} CCF &= \exp(-SS) && \text{For a beam neutron flux type} \\ CCF &= E_2(SS) && \text{For an isotropic neutron flux type; the } E_2(x) \text{ function is defined in Equations 43 and 44} \end{aligned} \tag{42}$$

$$E_2(x) = e^{-x}\left(1 - \frac{x^2 + 2.334733\,x + 0.250621}{x^2 + 3.330657\,x + 1.681534}\right) \qquad x > 1 \tag{43}$$

$$\begin{aligned} R &= 0.00107857\,x^5 - 0.00976004\,x^4 + 0.05519968\,x^3 - 0.24991055\,x^2 \\ &\quad + 0.99999193\,x - 0.57721566 \\ E_2(x) &= e^{-x} - xR + x\ln(x) \end{aligned} \qquad 0 < x \le 1 \tag{44}$$

Table 10. *Cover material data applied by STAYSL PNNL.*

Cover Material	Cover Code	Density [a] (g/cm^3)	Atomic Mass [b] (g/mol)
Boron	BORO	2.34	10.811
Cadmium	CADM	8.69	112.411
Gadolinium	GADO	7.90	157.25
Gold	GOLD	19.3	196.966569

[a] From Table 2 in Appendix 2 of Yaws [54] for pure elements.
[b] From Wieser and Berglund [51].

Within STASYL PNNL, self-shielding and cover corrections are applied to the neutron activation cross sections prior to the least-squares spectral adjustment (the activities, however, are not modified by the software).

8.5.2 Covariance Values

It is recommended that covariances be fully specified for all input data, including cross sections, activities, and the input flux spectrum.

The nuclear cross section covariances (adopted from the IRDF-2002 library) are automatically included (and cannot be changed by the user). While IRDF-2002 does contain some information on the cross section correlations between different reactions, not all reactions supported by STAYSL PNNL have data and thus a general approach using IRDF-2002 is not feasible. STAYSL PNNL takes the approach of applying a user-specified, fixed cross correlation value in the FS parameter (see Record 3 in Table 7). This cross corellation value is uniformly applied for all off-diagonal elements of the reaction-by-reaction cross section covariance matrix (while the diagonal elements are derived from the IRDF-2002 cross section covariances).

For activities, the ACVX parameter of Record 3 (Table 7) is a flag to indicate whether to use a set of user-specified values or a uniform calculation for off-diagonal elements. When ACVX is less than zero, the user-supplied activity covariance matrix is read as input (see Record 7 in Table 7). Otherwise the off-diagonal elements of the activity covariance matrix are set equal to the square of the non-negative ACVX value (diagonal elements are based on the SDA reaction rate uncertainties specified in Record 5 of the input).

Covariances for the initial flux spectrum can be provided as input (see Record 14 in Table 7). However, flux covariances are, unfortunately, only rarely available because neutron calculations (such as from the MCNP computer code) do not provide such information. Consequently, STAYSL PNNL allows the user to specify parameters for a Gaussian flux covariance function on the assumption that nearby flux groups are strongly correlated, whereas widely separated flux groups have weak or no correlation. This approximation is analogous to smoothing functions used in prior neutron spectral unfolding computer codes where iterations on the neutron flux were smoothed to prevent unphysical flux solutions. The user must determine if the use of a

Gaussian covariance function is appropriate or not (if not, then external calculations would be required to generate flux covariance data to put in the run parameters input file).

The Gaussian formalism for calculating flux covariance is turned on by entering a positive value for the FCHN parameter (see Record 3 in Table 7), which equates to the "full width at half maximum" of short range Gaussian covariance for flux. Long range flux covariance is entered as the value for the FCVX parameter (also in Record 3). The flux covariance between energy groups *i* and *j* ($FCOV_{i,j}$) is calculated as shown in Equations 45 and 46 from the values for FCVX, FCHN, and FERR (see Records 10 and 12 in Table 7). The $\frac{1}{2}\cdot\sqrt{2}$ term is a normalization factor set such that the maximum correlation allowed between flux groups is 100%. As noted in Equation 46, application of the Gaussian formula is limited to the cases where the difference in energy group numbers is less than or equal to the integral value of 3 times *FCHN*.

$$FCOV_{i,i} = FCVX^2 + (1.0 - FCVX^2)\cdot FERR_i^2 \qquad \text{i = j} \qquad (45)$$

$$FCOV_{i,j} = FCVX^2 + (1.0 - FCVX^2)\cdot\left[\exp\left[-\left(\frac{\frac{\sqrt{2}}{2}\cdot(|i-j|)}{FCHN}\right)^2\right]\right]^2 \cdot FERR_i \cdot FERR_j \qquad \text{i ≠ j and } |i-j| \le [3\times FCHN] \qquad (46)$$

$$FCOV_{i,j} = FCVX^2 \qquad \text{i ≠ j and } |i-j| > [3\times FCHN]$$

8.5.3 Specifying the Low-Energy Input Neutron Spectrum

Calculations of the neutron spectrum for nuclear reactors don't always extend to thermal neutron energies or may not provide adequate detail for the accurate determination of reaction rates in the thermal and resonance energy regions. STAYSL PNNL thus provides an option (via the ITHERM parameter in input Record 16) to calculate the neutron flux below a user specified neutron energy by assuming a 1/E slowing down spectrum in the resonance region and a thermal Maxwellian distribution in the thermal region. The neutron flux below the lowest user-specified energy, E_{low}, is calculated using Equation 47. Between a user-specified inverse joining energy, *ETE*, and E_{low} the neutron flux is proportional to the inverse energy. Below *ETE*, a thermal Maxwellian function is used to calculate the flux for the operating temperature of the reactor (*TMPR*; see Table 7).

$$Flux_i = \frac{B}{E_i}$$

for the ith energy group, where where $ETE \le E_i < E_{low}$ and B is determined by back-calculating with this equation from the known flux at $E_i = E_{low}$

or (47)

$$Flux_i = A\cdot E_i \cdot \exp\left(\frac{-E_i}{TMPR}\right)$$

for the ith energy group, where $E_i < ETE$ and A is determined by back-calculating with this equation from the known flux at $E_i = ETE$

8.5.4 Assumptions/Limitations

The following assumptions were used in the development of the STAYSL PNNL code.

- Available material/reaction pairs are those defined in Table 2.
- An application run uses an initial estimate of the neutron spectrum that is consistent with the data within the stated uncertainties on the neutron flux.
- An application run uses input activity (sig-phi) data that is accurate to within the stated uncertainties.
- A 100-group energy structure is sufficient/appropriate for the problem being evaluated (or the user is advanced enough to use NJOY99 and NJpp to build data libraries with a suitable energy grid structure).
- The cross section and covariance data libraries used for input do not include or require any spectral weighting (which is true of the default data libraries derived from IRDF-2002 data).
- The time and ACNM normalization are consistent, preferably having been defined in SigPhi Calculator.
- Neutron self-shielding was calculated correctly (i.e., with the SHIELD code) for relatively small flux monitor wires or foils where neutron scattering and flux depression effects are negligible.

It is important to start analysis with consistent activity (sig-phi) data based on properly calibrated instruments and appropriate measurement techniques. If one starts with incorrect data, then the output from STAYSL PNNL is likely to not make sense and give poor fits (such as very high chi-square values and large deviations between reactions).

STAYSL PNNL is best used for spectral adjustment to refine a reasonable estimate of the neutron spectrum, not as a tool to determine a completely unknown neutron spectrum.

The STAYSL PNNL suite using the IRDF-2002 data is limited to evaluations for neutrons below 20 MeV. For problems with neutrons above 20 MeV, different cross section and covariance libraries are required. Note that it expected to be possible to expand the cross section and covariance information given the recent release of the IRDFF library [22].

STAYSL PNNL is limited to using four cover materials (boron, cadmium, gadolinium, and gold).

The mini-spectrum output is a collapsed representation provided for user convenience in diagnostic assessment of the output or as an aid to more compact reporting of the results.

9.0 SPECTER

9.1 Introduction/Background/Purpose

SPECTER [83, 84, 85] is a Fortran-based computer code associated with STAYSL PNNL, but not included in the STAYSL PNNL suite. SPECTER is thus briefly described here for the convenience of the reader. The SPECTER computer code performs radiation damage [e.g., 86, 87, 88] calculations using the adjusted neutron spectrum and covariances determined as the output of STAYSL PNNL. STAYSL PNNL generates an output file named "sta_dam.dat" whenever it is executed (except for a FIR run or activity run), and this file comprises the input to SPECTER.

Neutron radiation damage in materials results from nuclear collisions and reactions which produce energetic recoil atoms of the host material or reaction products. These recoiling atoms then generate electronic excitations in the host material (electronic energy loss) and elastic and inelastic collision events (nuclear energy loss) that sometimes result in displacing additional host atoms. SPECTER calculates the displacement damage resulting from nuclear energy loss events.

The SPECTER computer code has been written to facilitate damage calculations for any specified neutron irradiation. To run SPECTER, a user need only specify the neutron flux spectrum. The code will then convert the required libraries of displacement cross sections, recoil distributions, and other nuclear data into the user's group structure and will proceed to perform spectral averaging using those quantities. SPECTER calculates spectral-averaged displacements, recoil spectra, gas production, and total damage energy (Kerma) for 41 pure elements. SPECTER also includes the additional non-linear production of helium and dpa from the two-step 58Ni(n,g)59Ni(n,He) reaction [89]. Output from SPECTER can be used with the related code SPECOMP [90] to determine displacement damage for alloys, insulators, and breeder materials.

10.0 References

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Appendix A: MAT Numbers

Appendix A

MAT Numbers

Table A.1 lists selected nuclides and the associated MAT number based on ENDF/B-VI and ENDF/B-VII indexes compiled by the NJOY99 developers at Los Alamos National Laboratory [64, 65, 66]. Other data libraries (e.g., JENDL, JEFF, etc.) may use different numbers. These values are used by convention, but are not mandatory. The ZA and LISO (sometimes referred to as LIS0) parameters [45] can be used to confirm that the data is for the entity of interest. Note that nuclides listed in the table as Z-Cc-nat (where Z is the atomic number and Cc is the element symbol) are sometimes referred to as Z-CC-0.

Table A.1. *Compilation of MAT numbers corresponding to selected nuclides.*

Nuclide	MAT #	Nuclide	MAT #	Nuclide	MAT #	Nuclide	MAT #	Nuclide	MAT #
1-H-1	125	18-Ar-38	1831	28-Ni-60	2831	36-Kr-85	3646	44-Ru-99	4434
1-H-2	128	18-Ar-40	1837	28-Ni-61	2834	36-Kr-86	3649	44-Ru-100	4437
1-H-3	131	19-K-nat	1900	28-Ni-62	2837	37-Rb-85	3725	44-Ru-101	4440
2-He-3	225	19-K-39	1925	28-Ni-64	2843	37-Rb-86	3728	44-Ru-102	4443
2-He-4	228	19-K-40	1928	29-Cu-63	2925	37-Rb-87	3731	44-Ru-103	4446
3-Li-6	325	19-K-14	1931	29-Cu-65	2931	38-Sr-84	3825	44-Ru-104	4449
3-Li-7	328	20-Ca-nat	2000	30-Zn-nat	3000	38-Sr-86	3831	44-Ru-105	4452
4-Be-7	419	20-Ca-40	2025	30-Zn-64	3025	38-Sr-87	3834	44-Ru-106	4455
4-Be-9	425	20-Ca-42	2031	30-Zn-66	3031	38-Sr-88	3837	45-Rh-103	4525
5-B-10	525	20-Ca-43	2034	30-Zn-67	3034	38-Sr-89	3840	45-Rh-105	4531
5-B-11	528	20-Ca-44	2037	30-Zn-68	3037	38-Sr-90	3843	46-Pd-102	4625
6-C-nat	600	20-Ca-46	2043	30-Zn-70	3043	39-Y-89	3925	46-Pd-104	4631
7-N-14	725	20-Ca-48	2049	31-Ga-nat	3100	39-Y-90	3928	46-Pd-105	4634
7-N-15	728	21-Sc-45	2125	31-Ga-69	3125	39-Y-91	3931	46-Pd-106	4637
8-O-16	825	22-Ti-nat	2200	31-Ga-71	3131	40-Zr-nat	4000	46-Pd-107	4640
8-O-17	828	22-Ti-46	2225	32-Ge-70	3225	40-Zr-90	4025	46-Pd-108	4643
9-F-19	925	22-Ti-47	2228	32-Ge-72	3231	40-Zr-91	4028	46-Pd-110	4649
11-Na-22	1122	22-Ti-48	2231	32-Ge-73	3234	40-Zr-92	4031	47-Ag-107	4725
11-Na-23	1125	22-Ti-49	2234	32-Ge-74	3237	40-Zr-93	4034	47-Ag-109	4731
12-Mg-nat	1200	22-Ti-50	2237	32-Ge-76	3243	40-Zr-94	4037	47-Ag-110m	4735
12-Mg-24	1225	23-V-nat	2300	33-As-74	3322	40-Zr-95	4040	47-Ag-111	4737
12-Mg-25	1228	23-V-50	2325	33-As-75	3325	40-Zr-96	4043	48-Cd-nat	4800
12-Mg-26	1231	23-V-51	2328	34-Se-74	3425	41-Nb-93	4125	48-Cd-106	4825
13-Al-27	1325	24-Cr-50	2425	34-Se-75	3428	41-Nb-94	4128	48-Cd-108	4831
14-Si-28	1425	24-Cr-52	2431	34-Se-76	3431	41-Nb-95	4131	48-Cd-110	4837
14-Si-29	1428	24-Cr-53	2434	34-Se-77	3434	42-Mo-nat	4200	48-Cd-111	4840
14-Si-30	1431	24-Cr-54	2437	34-Se-78	3437	42-Mo-92	4225	48-Cd-112	4843
15-P-31	1525	25-Mn-55	2525	34-Se-79	3440	42-Mo-94	4231	48-Cd-113	4846
16-S-nat	1600	26-Fe-54	2625	34-Se-80	3443	42-Mo-95	4234	48-Cd-113m	4847
16-S-32	1625	26-Fe-56	2631	34-Se-82	3449	42-Mo-96	4237	48-Cd-114	4849
16-S-33	1628	26-Fe-57	2634	35-Br-79	3525	42-Mo-97	4240	48-Cd-115m	4853
16-S-34	1631	26-Fe-58	2637	35-Br-81	3531	42-Mo-98	4243	48-Cd-116	4855
16-S-36	1637	27-Co-58	2722	36-Kr-78	3625	42-Mo-99	4246	49-In-nat	4900
17-Cl-nat	1700	27-Co-58m	2723	36-Kr-80	3631	42-Mo-100	4249	49-In-113	4925
17-Cl-35	1725	27-Co-59	2725	36-Kr-82	3637	43-Tc-99	4325	49-In-115	4931
17-Cl-37	1731	28-Ni-58	2825	36-Kr-83	3640	44-Ru-96	4425	50-Sn-112	5025
18-Ar-36	1825	28-Ni-59	2828	36-Kr-84	3643	44-Ru-98	4431	50-Sn-113	5028

Nuclide	MAT #
50-Sn-114	5031
50-Sn-115	5034
50-Sn-116	5037
50-Sn-117	5040
50-Sn-118	5043
50-Sn-119	5046
50-Sn-120	5049
50-Sn-122	5055
50-Sn-123	5058
50-Sn-124	5061
50-Sn-125	5064
50-Sn-126	5067
51-Sb-121	5125
51-Sb-123	5131
51-Sb-124	5134
51-Sb-125	5137
51-Sb-126	5140
52-Te-120	5225
52-Te-122	5231
52-Te-123	5234
52-Te-124	5237
52-Te-125	5240
52-Te-126	5243
52-Te-127m	5247
52-Te-128	5249
52-Te-129m	5253
52-Te-130	5255
52-Te-132	5261
53-I-127	5325
53-I-129	5331
53-I-130	5334
53-I-131	5337
53-I-135	5349
54-Xe-123	5422
54-Xe-124	5425
54-Xe-126	5431
54-Xe-128	5437
54-Xe-129	5440
54-Xe-130	5443
54-Xe-131	5446
54-Xe-132	5449
54-Xe-133	5452
54-Xe-134	5455
54-Xe-135	5458
54-Xe-137	5461
55-Cs-133	5525
55-Cs-134	5528
55-Cs-135	5531
55-Cs-136	5534
55-Cs-137	5537
56-Ba-130	5625

Nuclide	MAT #
56-Ba-132	5631
56-Ba-133	5634
56-Ba-134	5637
56-Ba-135	5640
56-Ba-136	5643
56-Ba-137	5646
56-Ba-138	5649
56-Ba-140	5655
57-La-138	5725
57-La-139	5728
57-La-140	5731
58-Ce-136	5825
58-Ce-138	5831
58-Ce-139	5834
58-Ce-140	5837
58-Ce-141	5840
58-Ce-142	5843
58-Ce-143	5846
58-Ce-144	5849
59-Pr-141	5925
59-Pr-142	5928
59-Pr-143	5931
60-Nd-142	6025
60-Nd-143	6028
60-Nd-144	6031
60-Nd-145	6034
60-Nd-146	6037
60-Nd-147	6040
60-Nd-148	6043
60-Nd-150	6049
61-Pm-147	6149
61-Pm-148	6152
61-Pm-148m	6153
61-Pm-149	6155
61-Pm-151	6161
62-Sm-144	6225
62-Sm-147	6234
62-Sm-148	6237
62-Sm-149	6240
62-Sm-150	6243
62-Sm-151	6246
62-Sm-152	6249
62-Sm-153	6252
62-Sm-154	6255
63-Eu-151	6325
63-Eu-152	6328
63-Eu-153	6331
63-Eu-154	6334
63-Eu-155	6337
63-Eu-156	6340
63-Eu-157	6343

Nuclide	MAT #
64-Gd-152	6425
64-Gd-153	6428
64-Gd-154	6431
64-Gd-155	6434
64-Gd-156	6437
64-Gd-157	6440
64-Gd-158	6443
64-Gd-160	6449
65-Tb-159	6525
65-Tb-160	6528
66-Dy-156	6625
66-Dy-158	6631
66-Dy-160	6637
66-Dy-161	6640
66-Dy-162	6643
66-Dy-163	6646
66-Dy-164	6649
67-Ho-165	6725
67-Ho-166m	6729
68-Er-162	6825
68-Er-164	6831
68-Er-166	6837
68-Er-167	6840
68-Er-168	6843
68-Er-170	6849
69-Tm-168	6922
69-Tm-169	6925
69-Tm-170	6928
71-Lu-175	7125
71-Lu-176	7128
72-Hf-nat	7200
72-Hf-174	7225
72-Hf-176	7231
72-Hf-177	7234
72-Hf-178	7237
72-Hf-179	7240
72-Hf-180	7243
73-Ta-180	7325
73-Ta-181	7328
73-Ta-182	7331
74-W-nat	7400
74-W-180	7425
74-W-182	7431
74-W-183	7434
74-W-184	7437
74-W-186	7443
75-Re-185	7525
75-Re-187	7531
77-Ir-191	7725
77-Ir-193	7731
79-Au-197	7925

Nuclide	MAT #
80-Hg-196	8025
80-Hg-198	8031
80-Hg-199	8034
80-Hg-200	8037
80-Hg-201	8040
80-Hg-202	8043
80-Hg-204	8049
81-Tl-203	8125
81-Tl-205	8131
82-Pb-204	8225
82-Pb-206	8231
82-Pb-207	8234
82-Pb-208	8237
83-Bi-209	8325
88-Ra-223	8825
88-Ra-224	8828
88-Ra-225	8831
88-Ra-226	8834
89-Ac-225	8925
89-Ac-226	8928
89-Ac-227	8931
90-Th-227	9025
90-Th-228	9028
90-Th-229	9031
90-Th-230	9034
90-Th-232	9040
90-Th-233	9043
90-Th-234	9046
91-Pa-229	9125
91-Pa-230	9128
91-Pa-231	9131
91-Pa-232	9134
91-Pa-233	9137
92-U-230	9213
92-U-232	9216
92-U-232	9219
92-U-233	9222
92-U-234	9225
92-U-235	9228
92-U-236	9231
92-U-237	9234
92-U-238	9237
92-U-239	9240
92-U-240	9243
92-U-241	9246
93-Np-234	9337
93-Np-235	9340
93-Np-236	9343
93-Np-237	9346
93-Np-238	9349
93-Np-239	9352

Nuclide	MAT #
94-Pu-236	9428
94-Pu-237	9431
94-Pu-238	9434
94-Pu-239	9437
94-Pu-240	9440
94-Pu-241	9443
94-Pu-242	9446
94-Pu-243	9449
94-Pu-244	9452
94-Pu-246	9458
95-Am-241	9543
95-Am-242	9546
95-Am-242m	9547
95-Am-243	9549
95-Am-244	9552
95-Am-244m	9553
96-Cm-240	9625
96-Cm-241	9628
96-Cm-242	9631
96-Cm-243	9634
96-Cm-244	9637
96-Cm-245	9640
96-Cm-246	9643
96-Cm-247	9646
96-Cm-248	9649
96-Cm-249	9652
96-Cm-250	9655
97-Bk-245	9740
97-Bk-246	9743
97-Bk-247	9746
97-Bk-248	9749
97-Bk-249	9752
97-Bk-250	9755
98-Cf-246	9843
98-Cf-248	9849
98-Cf-249	9852
98-Cf-250	9855
98-Cf-251	9858
98-Cf-252	9861
98-Cf-253	9864
98-Cf-254	9867
99-Es-251	9911
99-Es-252	9912
99-Es-253	9913
99-Es-254	9914
99-Es-254m	9915
99-Es-255	9916
100-Fm-255	9936

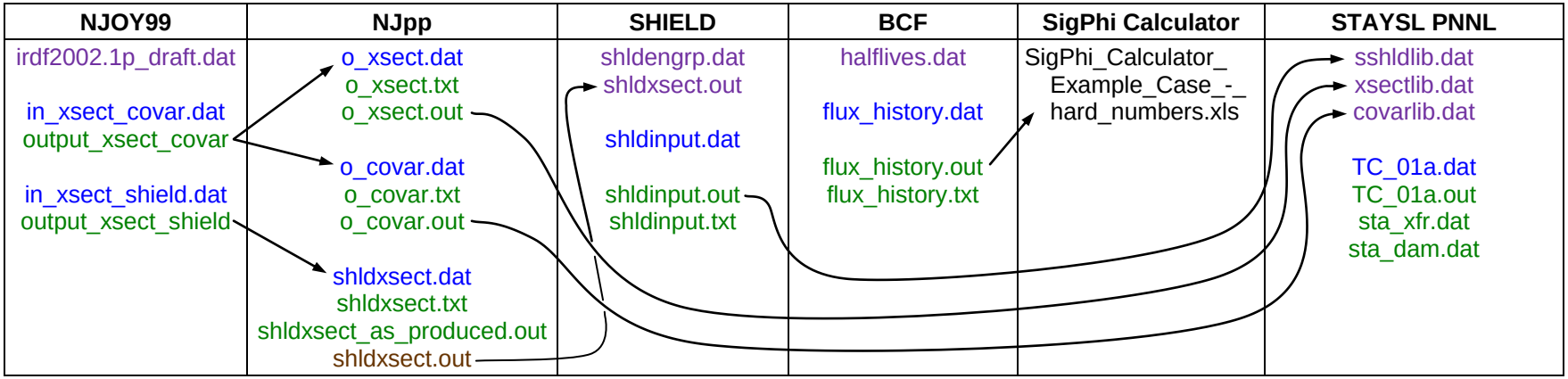
Appendix B: File Content Information and Example Cases

Appendix B

File Content Information and Example Cases

List of Test Case Files

A set of example files is packaged for distribution with the STAYSL PNNL software suite. These files provide examples of the input and output file structure and also provide a baseline for the user to compare against when performing runs on their own installation of the software. The NJOY and NJpp input/output files result in valid library files, but otherwise the examples are contrived and should not be used for any meaningful purpose. The function is really to show file structure and demonstrate the software functionality. For each software program, test case files are listed in the table below and consist of ***library files***, ***run parameter input files***, and ***output files*** (color-coded accordingly, except for the SigPhi calculator file, which contains all three types of information). One file that differs in how it was produced is the ***shldxsect.out*** file, which was obtained by manually editing the NJpp output to remove extraneous reactions not used by SHIELD. Arrows in the table show where the output from one code feeds into another code as input (usually with a file name change).



NJOY99 Input for Extracting Cross Section/Cross Section Covariance Data for STAYSL PNNL

The listing below shows the input to NJOY99 to obtain cross section and cross section covariance data from the IRDF-2002 library. Because the energy grid block (marked in green text) is repeated multiple times, that block is replaced with {energy grid} after the first instance in the interest of conciseness in this appendix.

```
moder
 20 -21 /
reconr
 -21 -22 /
 'PENDF for data from IRDF 2002' /
 325 /
 .10 /
 500 /
 .10 /
 525 /
 .10 /
 925 /
 .10 /
 1125 /
 .10 /
 1225 /
 .10 /
 1325 /
 .10 /
 1525 /
 .10 /
 1625 /
 .10 /
 2126 /
 .10 /
 2225 /
 .10 /
 2228 /
 .10 /
 2231 /
 .10 /
 2234 /
 .10 /
 2328 /
 .10 /
 2431 /
```

Continued in next column ⮎

```
 .10 /
 2525 /
 .10 /
 2625 /
 .10 /
 2631 /
 .10 /
 2637 /
 .10 /
 2725 /
 .10 /
 2825 /
 .10 /
 2831 /
 .10 /
 2925 /
 .10 /
 2931 /
 .10 /
 3025 /
 .10 /
 3325 /
 .10 /
 3925 /
 .10 /
 4025 /
 .10 /
 4125 /
 .10 /
 4525 /
 .10 /
 4731 /
 .10 /
 4800 /
 .10 /
 4931 /
```

Continued in next column ⮎

```
 .10 /
 5325 /
 .10 /
 5728 /
 .10 /
 5925 /
 .10 /
 6400 /
 .10 /
 6925 /
 .10 /
 7328 /
 .10 /
 7443 /
 .10 /
 7925 /
 .10 /
 8034 /
 .10 /
 8225 /
 .10 /
 9040 /
 .10 /
 9228 /
 .10 /
 9237 /
 .10 /
 9346 /
 .10 /
 9437 /
 .10 /
 9543 /
 .10 /
 0 /
```

Continued on next page ⮑

```
 broadr / Doppler broaden XS
  -21 -22 -23 /
  325 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  325 1 0 2 0 1 1 1 /
  '3-Li-6 (N,A)' /
  300. /
  1.e+10 /
  100 /
  1.0000E-04 1.0000E-03 1.0000E-02 2.3000E-02 5.0000E-02 7.6000E-02 1.1500E-01
  1.7000E-01 2.5500E-01 3.8000E-01 5.5000E-01 8.4000E-01 1.2750E+00 1.9000E+00
  2.8000E+00 4.2500E+00 6.3000E+00 9.2000E+00 1.3500E+01 2.1000E+01 3.0000E+01
  4.5000E+01 6.9000E+01 1.0000E+02 1.3500E+02 1.7000E+02 2.2000E+02 2.8000E+02
  3.6000E+02 4.5000E+02 5.7500E+02 7.6000E+02 9.6000E+02 1.2750E+03 1.6000E+03
  2.0000E+03 2.7000E+03 3.4000E+03 4.5000E+03 5.5000E+03 7.2000E+03 9.2000E+03
  1.2000E+04 1.5000E+04 1.9000E+04 2.5500E+04 3.2000E+04 4.0000E+04 5.2500E+04
  6.6000E+04 8.8000E+04 1.1000E+05 1.3500E+05 1.6000E+05 1.9000E+05 2.2000E+05
  2.5500E+05 2.9000E+05 3.2000E+05 3.6000E+05 4.0000E+05 4.5000E+05 5.0000E+05
  5.5000E+05 6.0000E+05 6.6000E+05 7.2000E+05 7.8000E+05 8.4000E+05 9.2000E+05
  1.0000E+06 1.2000E+06 1.4000E+06 1.6000E+06 1.8000E+06 2.0000E+06 2.3000E+06
  2.6000E+06 2.9000E+06 3.3000E+06 3.7000E+06 4.1000E+06 4.5000E+06 5.0000E+06
  5.5000E+06 6.0000E+06 6.7000E+06 7.4000E+06 8.2000E+06 9.0000E+06 1.0000E+07
  1.1000E+07 1.2000E+07 1.3000E+07 1.4000E+07 1.5000E+07 1.6000E+07 1.7000E+07
  1.8000E+07 1.9000E+07 2.0000E+07 /
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  325 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
```

Continued on next page ⤳

```
 broadr / Doppler broaden XS
  -21 -22 -23 /
  500 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  500 1 0 2 0 1 1 1 /
  '5-B-0 (N,A)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 broadr / Doppler broaden XS
  -21 -22 -23 /
  525 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  525 1 0 2 0 1 1 1 /
  '5-B-10 (N,A)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  525 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
```

Continued in next column ⮣

```
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  925 1 0 2 0 1 1 1 /
  '9-F-19 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  925 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  1125 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  1125 1 0 2 0 1 1 1 /
  '11-Na-23 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  1125 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  1225 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
```

Continued in next column ⮣

```
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  1225 1 0 2 0 1 1 1 /
  '12-Mg-24 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  1225 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  1325 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  1325 1 0 2 0 1 1 1 /
  '13-Al-27 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  1325 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  1525 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
```

Continued on next page ⮧

```
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  1525 1 0 2 0 1 1 1 /
  '15-P-31 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  1525 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  1625 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  1625 1 0 2 0 1 1 1 /
  '16-S-32 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  1625 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2225 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
```

Continued in next column ⮣

```
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2225 1 0 2 0 1 1 1 /
  '22-Ti-46 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2225 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2228 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2228 1 0 2 0 1 1 1 /
  '22-Ti-47 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2228 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2228 1 0 2 0 1 1 1 /
  '22-Ti-47 (N,X)' /
  300. /
  1.e+10 /
  100 /
```

Continued in next column ⮣

```
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2228 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2231 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2231 1 0 2 0 1 1 1 /
  '22-Ti-48 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2231 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2231 1 0 2 0 1 1 1 /
  '22-Ti-48 (N,X)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2231 1 2 1 1 /
```

Continued on next page ⮧

```
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2234 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2234 1 0 2 0 1 1 1 /
  '22-Ti-49 (N,X)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2234 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2328 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2328 1 0 2 0 1 1 1 /
  '23-V-51 (N,A)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2328 1 2 1 1 /
  0 33 /
```

Continued in next column ⮣

```
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2431 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2431 1 0 2 0 1 1 1 /
  '24-Cr-52 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2431 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2525 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2525 1 0 2 0 1 1 1 /
  '25-Mn-55 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2525 1 2 1 1 /
  0 33 /
  100 /
```

Continued in next column ⮣

```
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2625 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2625 1 0 2 0 1 1 1 /
  '26-Fe-54 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2625 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2631 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2631 1 0 2 0 1 1 1 /
  '26-Fe-56 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2631 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
```

Continued on next page ⮧

```
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2637 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2637 1 0 2 0 1 1 1 /
  '26-Fe-58 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2637 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2725 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2725 1 0 2 0 1 1 1 /
  '27-Co-59 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2725 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
```

Continued in next column ⮣

```
  -21 -22 -23 /
  2825 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2825 1 0 2 0 1 1 1 /
  '28-Ni-58 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2825 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2831 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2831 1 0 2 0 1 1 1 /
  '28-Ni-60 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2831 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
```

Continued in next column ⮣

```
  2925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2925 1 0 2 0 1 1 1 /
  '29-Cu-63 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2925 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2931 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2931 1 0 2 0 1 1 1 /
  '29-Cu-65 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2931 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  3025 1 0 0 0. /
```

Continued on next page ⮧

```
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  3025 1 0 2 0 1 1 1 /
  '30-Zn-64 (N,P)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  3025 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  3325 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  3325 1 0 2 0 1 1 1 /
  '33-As-75 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  3325 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  3925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
```

Continued in next column ⮣

```
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  3925 1 0 2 0 1 1 1 /
  '39-Y-89 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  3925 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4025 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4025 1 0 2 0 1 1 1 /
  '40-Zr-90 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4025 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4125 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
```

Continued in next column ⮣

```
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4125 1 0 2 0 1 1 1 /
  '41-Nb-93 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4125 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4125 1 0 2 0 1 1 1 /
  '41-Nb-93 (N,N'')' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4125 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4525 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4525 1 0 2 0 1 1 1 /
  '45-Rh-103 (N,N'')' /
  300. /
  1.e+10 /
```

Continued on next page ⮧

```
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4525 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4731 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4731 1 0 2 0 1 1 1 /
  '47-Ag-109 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4731 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4800 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4800 1 0 2 0 1 1 1 /
  '48-Cd-0 (N,G)' /
  300. /
  1.e+10 /
  100 /
```

Continued in next column ⮣

```
{energy grid}
  3 /
  0 /
  0 /
 broadr / Doppler broaden XS
  -21 -22 -23 /
  4931 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  4931 1 0 2 0 1 1 1 /
  '49-In-115 (N,N'')' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  4931 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  5325 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  5325 1 0 2 0 1 1 1 /
  '53-I-127 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  5325 1 2 1 1 /
```

Continued in next column ⮣

```
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  5728 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  5728 1 0 2 0 1 1 1 /
  '57-La-139 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  5728 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  5925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  5925 1 0 2 0 1 1 1 /
  '59-Pr-141 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  5925 1 2 1 1 /
  0 33 /
```

Continued on next page ⮧

```
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  6400 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  6400 1 0 2 0 1 1 1 /
  '64-Gd-0 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 broadr / Doppler broaden XS
  -21 -22 -23 /
  6925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  6925 1 0 2 0 1 1 1 /
  '69-Tm-169 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  6925 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  7328 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
```

Continued in next column ⮣

```
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  7328 1 0 2 0 1 1 1 /
  '73-Ta-181 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  7328 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  7443 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  7443 1 0 2 0 1 1 1 /
  '74-W-186 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  7443 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  7925 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
```

Continued in next column ⮣

```
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  7925 1 0 2 0 1 1 1 /
  '79-Au-197 (N,2N)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  7925 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  8034 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  8034 1 0 2 0 1 1 1 /
  '80-Hg-199 (N,N'')' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  8034 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  8225 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
```

Continued on next page ⮧

```
  -21 -23 0 31 /
  8225 1 0 2 0 1 1 1 /
  '82-Pb-204 (N,N'')' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  10 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  8225 1 2 1 1 /
  0 40 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9040 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  9040 1 0 2 0 1 1 1 /
  '90-Th-232 (N,F)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9040 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9228 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
```

Continued in next column ⮣

```
  9228 1 0 2 0 1 1 1 /
  '92-U-235 (N,F)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9228 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9237 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  9237 1 0 2 0 1 1 1 /
  '92-U-238 (N,F)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9237 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9346 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  9346 1 0 2 0 1 1 1 /
```

Continued in next column ⮣

```
  '93-Np-237 (N,F)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9346 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9437 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  9437 1 0 2 0 1 1 1 /
  '94-Pu-239 (N,F)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9437 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  9543 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  9543 1 0 2 0 1 1 1 /
  '95-Am-241 (N,F)' /
```

Continued on next page ⮡

```
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  9543 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 broadr / Doppler broaden XS
  -21 -22 -23 /
  2126 1 0 0 0. /
  0.001 2.0e+6 0.003 /
  300. /
  0 /
 groupr / Prepare multigroup XS
  -21 -23 0 31 /
  2126 1 0 2 0 1 1 1 /
  '21-Sc-45 (N,G)' /
  300. /
  1.e+10 /
  100 /
{energy grid}
  3 /
  0 /
  0 /
 errorr / Prepare rel. covariance
  -21 -22 31 32 0 0 /
  2126 1 2 1 1 /
  0 33 /
  100 /
{energy grid}
 stop
```

STAYSL PNNL Extended Output (IPNT=0)

The listing below shows the output file contents and structure for an arbitrary normal STAYSL PNNL run example. The first block is an echo of the input file. This is the extended output, so the output includes extra information (e.g., cross sections, correlation matrices) that is not included with normal output (IPNT=1).

```
Case1, Sample A (138.79 EFPD)
  100    6    0    0    1
   0.00500   9.00000   0.03000   0.00100
   1.0500000   0   0 1.19931840E+07   1.0000000
FE54P    4.587E-12 0.030       0.00       0.00        (    )
FE58G    1.104E-10 0.030       0.00       0.00        (    )
NB93N    1.085E-11 0.050       0.00       0.00        (    )
NB93G    2.013E-10 0.030       0.00       0.00        (    )
TI46P    6.118E-13 0.030       0.00       0.00        (    )
CO59G    3.410E-09 0.030       0.00       0.00        (    )
Flux Uncertainty
   4
 9.9000E-11 1.0000E-02 1.5000E+00 2.0100E+01
 6.0000E-01 1.5000E-01 1.5000E-01 1.5000E-01
Input Flux Spectrum
 101   0 4.200E+18 2.000E+01 5.000E-08
 1.0000E-11 3.0900E-10 3.9700E-10 5.1000E-10 6.5400E-10 8.4000E-10 1.0800E-09
 1.3900E-09 1.7800E-09 2.2800E-09 2.9300E-09 3.7700E-09 4.8400E-09 6.2100E-09
 7.9700E-09 1.0200E-08 1.3100E-08 1.6900E-08 2.1700E-08 2.7800E-08 3.5700E-08
 4.5900E-08 5.8900E-08 7.5600E-08 9.7100E-08 1.2500E-07 1.6000E-07 2.0600E-07
 2.6400E-07 3.3900E-07 4.3500E-07 5.5900E-07 7.1800E-07 9.2100E-07 1.1800E-06
 1.5200E-06 1.9500E-06 2.5100E-06 3.2200E-06 4.1300E-06 5.3000E-06 6.8100E-06
 8.7400E-06 1.1200E-05 1.4400E-05 1.8500E-05 2.3800E-05 3.0500E-05 3.9200E-05
 5.0300E-05 6.4600E-05 8.2900E-05 1.0700E-04 1.3700E-04 1.7600E-04 2.2500E-04
 2.9000E-04 3.7200E-04 4.7700E-04 6.1300E-04 7.8700E-04 1.0100E-03 1.3000E-03
 1.6700E-03 2.1400E-03 2.7500E-03 3.5300E-03 4.5300E-03 5.8100E-03 7.4700E-03
 9.5900E-03 1.2300E-02 1.5800E-02 2.0300E-02 2.6100E-02 3.3500E-02 4.3000E-02
 5.5200E-02 7.0800E-02 9.1000E-02 1.1700E-01 1.5000E-01 1.9300E-01 2.4700E-01
 3.1800E-01 4.0800E-01 5.2300E-01 6.7200E-01 8.6300E-01 1.1100E+00 1.4200E+00
 1.8300E+00 2.3500E+00 3.0100E+00 3.8700E+00 4.9700E+00 6.3800E+00 8.1900E+00
 1.0500E+01 1.3500E+01 1.7300E+01 2.0000E+01
 1.6270E-09 9.4330E-10 1.5000E-09 2.5870E-09 6.0030E-09 1.0220E-08 1.3620E-08
 2.4690E-08 3.5100E-08 6.6800E-08 1.7230E-07 1.7430E-07 2.6050E-07 4.6680E-07
 7.3500E-07 1.2690E-06 1.5450E-06 2.2430E-06 3.3060E-06 3.8620E-06 4.8710E-06
 5.3200E-06 4.9470E-06 4.4640E-06 3.1550E-06 2.1730E-06 1.3760E-06 1.0140E-06
 8.6900E-07 8.2500E-07 7.9600E-07 7.8100E-07 7.5600E-07 7.1500E-07 7.2600E-07
 7.0600E-07 7.0300E-07 6.9600E-07 6.9100E-07 6.8600E-07 6.7300E-07 6.8400E-07
 6.8200E-07 6.8900E-07 6.9400E-07 6.7700E-07 6.9600E-07 6.9400E-07 6.9500E-07
 6.9000E-07 6.9500E-07 7.0700E-07 6.9400E-07 7.0500E-07 7.0400E-07 7.1200E-07
 7.1700E-07 7.1100E-07 7.1300E-07 7.2100E-07 7.1800E-07 7.2400E-07 7.2000E-07
 7.3800E-07 7.4400E-07 7.3700E-07 7.5200E-07 7.6800E-07 7.6600E-07 7.7200E-07
 7.8400E-07 8.0700E-07 8.2200E-07 8.5500E-07 9.0300E-07 9.0000E-07 9.7600E-07
 1.0300E-06 1.0600E-06 1.1460E-06 1.2670E-06 1.3380E-06 1.4980E-06 1.6840E-06
 1.8000E-06 1.9530E-06 1.8190E-06 2.2390E-06 2.0780E-06 2.3120E-06 2.4390E-06
 2.1030E-06 1.5180E-06 1.0310E-06 7.7800E-07 4.1710E-07 1.7040E-07 4.7950E-08
 8.2560E-09 1.3215E-09 3.4500E-11
  10   13   28   11    8    5    8    7    5    5
```

```
                          ==============================
                                STAYSL PNNL OUTPUT
                          ==============================

STAYSL PNNL, version 1.0.1, 2012-Nov-30


SCENARIO TITLE: Case1, Sample A (138.79 EFPD)
--------------------------------------------------------------------------------
 NGROUP =   100    NRXN =     6    ACTIVITY NORM = 1.00000E+00

 COVARIANCE PARAMETERS (FCHN, FCVX, ACVX, FS)
   FLUXES:      WIDTH =  9.0000E+00   LONG RANGE COVAR. =  3.0000E-02
          ACTIVITIES =  5.0000E-03   X-SECT CROSS COR. =  1.0000E-03

   DETERM =   2.8200 × 10^  -3.00      ERROR =   0.0000E+00

 INPUT NORMALIZATION DATA
   AK1   =     1.05000     VAK        =     0.00090
   NORML =           0     RENORM     =     1.05000
   CHI²  =     2.68724     NORM. CHI² =     0.53745

 DOSIMETRY ACTIVITIES
    ──── INPUTS ─────  -UNADJUSTED FLUX-  — ADJUSTED FLUX —    CHI²  90% ACTIVITIES RANGE
RXN  MEASURED     ±%   ACTIVITY    %DIFF  ACTIVITY    %DIFF  CONTRIB --LOW E-- --HIGH E--   REACTION          CVR
 1  4.587E+12    3.00  4.396E+12   -4.16  4.556E+12   -0.69    0.221  2.00E+00  7.40E+00  FE54(N,P)MN54
 2  1.104E+14    3.00  2.183E+14   97.71  1.036E+14   -6.15   -1.011  1.00E-09  2.80E-04  FE58(N,G)FE59
 3  1.085E+13    5.00  1.023E+13   -5.75  1.077E+13   -0.76    0.138  7.20E-01  5.00E+00  NB93(N,N')NB93M
 4  2.013E+14    3.00  3.108E+14   54.39  2.056E+14    2.16    0.490  1.00E-08  1.90E-02  NB93(N,G)NB94
 5  6.118E+11    3.00  6.124E+11    0.09  6.175E+11    0.93    0.005  3.70E+00  9.00E+00  TI46(N,P)SC46
 6  3.410E+15    3.00  6.727E+15   97.27  3.420E+15    0.31    2.844  1.00E-09  1.00E-04  CO59(N,G)CO60

           % STD. DEV.  =         66.36               2.98

 DOSIMETRY DATA INPUT REL. CORRELATION MATRIX
       1    1000
       2      28    1000
       3      17      17    1000
       4      28      28      17    1000
       5      28      28      17      28    1000
       6      28      28      17      28      28    1000

 RELATIVE COV. MATRIX OF ACTIVITIES
      %         REL. CORRELATION MATRIX
  1 13.74     1000
  2 37.49       18    1000
  3 12.92      802      19    1000
  4 25.02       27     847      31    1000
  5 14.46      868      17     552      25    1000
  6 33.03       20     943      21     901      19    1000
```

CONTRIBUTION DUE TO INPUT FLUX COV. MATRIX

	%	REL. CORRELATION MATRIX					
1	13.58	1000					
2	35.43	19	1000				
3	12.61	832	20	1000			
4	23.01	30	975	34	1000		
5	14.10	901	18	579	28	1000	
6	33.02	20	998	22	981	19	1000

CONTRIBUTION DUE TO INPUT X-SEC. COV. MATRIX

	%	REL. CORRELATION MATRIX					
1	2.13	1000					
2	12.25	0	1000				
3	2.81	2	0	1000			
4	9.84	0	0	0	1000		
5	3.18	1	0	1	0	1000	
6	0.67	7	1	5	2	5	1000

INPUT DOSIMETRY X-SECTIONS

GRP	ENERGY	X-SECTIONS					
1	1.000E-10	0.0000E+00	9.9440E+00	0.0000E+00	8.7725E+00	0.0000E+00	2.8422E+02
2	1.000E-09	0.0000E+00	3.1445E+00	0.0000E+00	2.7792E+00	0.0000E+00	8.9881E+01
3	1.000E-08	0.0000E+00	1.6447E+00	0.0000E+00	1.4584E+00	0.0000E+00	4.7016E+01
4	2.300E-08	0.0000E+00	1.1030E+00	0.0000E+00	9.8188E-01	0.0000E+00	3.1539E+01
5	5.000E-08	0.0000E+00	8.2907E-01	0.0000E+00	7.4102E-01	0.0000E+00	2.3715E+01
6	7.600E-08	0.0000E+00	6.7331E-01	0.0000E+00	6.0421E-01	0.0000E+00	1.9266E+01
7	1.150E-07	0.0000E+00	5.5089E-01	0.0000E+00	4.9669E-01	0.0000E+00	1.5772E+01
8	1.700E-07	0.0000E+00	4.5124E-01	0.0000E+00	4.0949E-01	0.0000E+00	1.2929E+01
9	2.550E-07	0.0000E+00	3.6915E-01	0.0000E+00	3.3733E-01	0.0000E+00	1.0589E+01
10	3.800E-07	0.0000E+00	3.0482E-01	0.0000E+00	2.8106E-01	0.0000E+00	8.7611E+00
11	5.500E-07	0.0000E+00	2.4975E-01	0.0000E+00	2.3284E-01	0.0000E+00	7.1953E+00
12	8.400E-07	0.0000E+00	2.0243E-01	0.0000E+00	1.9140E-01	0.0000E+00	5.8575E+00
13	1.275E-06	0.0000E+00	1.6514E-01	0.0000E+00	1.5876E-01	0.0000E+00	4.8090E+00
14	1.900E-06	0.0000E+00	1.3569E-01	0.0000E+00	1.3295E-01	0.0000E+00	3.9874E+00
15	2.800E-06	0.0000E+00	1.1086E-01	0.0000E+00	1.1111E-01	0.0000E+00	3.3043E+00
16	4.250E-06	0.0000E+00	9.0600E-02	0.0000E+00	9.3200E-02	0.0000E+00	2.7578E+00
17	6.300E-06	0.0000E+00	7.4701E-02	0.0000E+00	7.9157E-02	0.0000E+00	2.3467E+00
18	9.200E-06	0.0000E+00	6.1749E-02	0.0000E+00	6.7724E-02	0.0000E+00	2.0324E+00
19	1.350E-05	0.0000E+00	5.0146E-02	0.0000E+00	5.7825E-02	0.0000E+00	1.7919E+00
20	2.100E-05	0.0000E+00	4.1165E-02	0.0000E+00	5.2096E-02	0.0000E+00	1.6666E+00
21	3.000E-05	0.0000E+00	3.3996E-02	0.0000E+00	7.5420E-01	0.0000E+00	1.6949E+00
22	4.500E-05	0.0000E+00	2.7613E-02	0.0000E+00	4.2915E-02	0.0000E+00	2.1147E+00
23	6.900E-05	0.0000E+00	2.2689E-02	0.0000E+00	2.8622E-01	0.0000E+00	4.4479E+00
24	1.000E-04	0.0000E+00	1.9308E-02	0.0000E+00	2.2314E+00	0.0000E+00	1.6355E+02
25	1.350E-04	0.0000E+00	1.7164E-02	0.0000E+00	4.3344E-02	0.0000E+00	4.7519E+01
26	1.700E-04	0.0000E+00	1.8017E-02	0.0000E+00	6.4538E+00	0.0000E+00	1.8550E+00
27	2.200E-04	0.0000E+00	4.6937E-01	0.0000E+00	3.4949E-01	0.0000E+00	4.6614E-01
28	2.800E-04	0.0000E+00	2.3082E+00	0.0000E+00	1.3140E+00	0.0000E+00	1.9255E-01
29	3.600E-04	0.0000E+00	2.2271E-01	0.0000E+00	4.4327E+00	0.0000E+00	1.0467E-01
30	4.500E-04	0.0000E+00	9.8447E-03	0.0000E+00	4.6378E-01	0.0000E+00	6.7590E-02
31	5.750E-04	0.0000E+00	8.0889E-03	0.0000E+00	1.7520E+00	0.0000E+00	4.6973E-02
32	7.600E-04	0.0000E+00	6.9786E-03	0.0000E+00	1.4875E+00	0.0000E+00	3.5727E-02
33	9.600E-04	0.0000E+00	6.0564E-03	0.0000E+00	3.9479E+00	0.0000E+00	2.8631E-02
34	1.275E-03	0.0000E+00	5.2855E-03	0.0000E+00	2.0784E+00	0.0000E+00	5.5084E-02
35	1.600E-03	0.0000E+00	4.6912E-03	0.0000E+00	1.3765E+00	0.0000E+00	2.1607E-02
36	2.000E-03	0.0000E+00	4.0926E-03	0.0000E+00	1.9197E+00	0.0000E+00	4.2080E-02
37	2.700E-03	0.0000E+00	3.6008E-03	0.0000E+00	7.7274E-01	0.0000E+00	1.4617E-01

38	3.400E-03	0.0000E+00	3.2551E-03	0.0000E+00	9.0917E-01	0.0000E+00	2.8668E-01
39	4.500E-03	0.0000E+00	3.1394E-03	0.0000E+00	6.2292E-01	0.0000E+00	3.2366E-01
40	5.500E-03	0.0000E+00	5.8630E-02	0.0000E+00	7.8424E-01	0.0000E+00	9.9886E-02
41	7.200E-03	0.0000E+00	7.5871E-03	0.0000E+00	5.5019E-01	0.0000E+00	7.1041E-02
42	9.200E-03	0.0000E+00	1.6421E-01	0.0000E+00	5.4198E-01	0.0000E+00	9.1808E-02
43	1.200E-02	0.0000E+00	3.4403E-03	0.0000E+00	4.7638E-01	0.0000E+00	4.8434E-02
44	1.500E-02	0.0000E+00	1.2141E-03	0.0000E+00	3.8777E-01	0.0000E+00	5.0166E-02
45	1.900E-02	0.0000E+00	8.9190E-03	0.0000E+00	3.4409E-01	0.0000E+00	3.6206E-02
46	2.550E-02	0.0000E+00	9.5364E-03	2.0557E-06	2.8654E-01	0.0000E+00	3.9667E-02
47	3.200E-02	0.0000E+00	1.0261E-02	5.4096E-05	2.4750E-01	0.0000E+00	2.3025E-02
48	4.000E-02	0.0000E+00	1.4419E-02	1.6471E-04	2.0416E-01	0.0000E+00	1.8720E-02
49	5.250E-02	0.0000E+00	5.2699E-03	3.1839E-04	1.6952E-01	0.0000E+00	1.9120E-02
50	6.600E-02	0.0000E+00	7.3899E-03	5.5691E-04	1.3984E-01	0.0000E+00	1.6554E-02
51	8.800E-02	0.0000E+00	8.7999E-03	8.5623E-04	1.1521E-01	0.0000E+00	1.7902E-02
52	1.100E-01	0.0000E+00	6.9811E-03	1.2999E-03	1.0049E-01	0.0000E+00	1.7644E-02
53	1.350E-01	0.0000E+00	9.1346E-03	1.7972E-03	9.1480E-02	0.0000E+00	1.5200E-02
54	1.600E-01	0.0000E+00	2.1465E-03	2.3442E-03	8.1565E-02	0.0000E+00	1.3495E-02
55	1.900E-01	0.0000E+00	4.8585E-03	2.9577E-03	7.2388E-02	0.0000E+00	1.2011E-02
56	2.200E-01	0.0000E+00	4.0539E-03	3.6813E-03	6.8375E-02	0.0000E+00	1.0908E-02
57	2.550E-01	0.0000E+00	5.0433E-03	4.4651E-03	6.4525E-02	0.0000E+00	1.0000E-02
58	2.900E-01	0.0000E+00	2.1602E-03	5.2301E-03	6.1402E-02	0.0000E+00	9.3374E-03
59	3.200E-01	0.0000E+00	3.1807E-03	6.2000E-03	5.9560E-02	0.0000E+00	8.8014E-03
60	3.600E-01	0.0000E+00	3.1884E-03	7.3192E-03	5.7593E-02	0.0000E+00	8.3075E-03
61	4.000E-01	0.0000E+00	3.1217E-03	8.9613E-03	5.5825E-02	0.0000E+00	7.8976E-03
62	4.500E-01	0.0000E+00	3.0553E-03	1.1126E-02	5.4299E-02	0.0000E+00	7.5327E-03
63	5.000E-01	0.0000E+00	3.0595E-03	1.3820E-02	5.2961E-02	0.0000E+00	7.2458E-03
64	5.500E-01	0.0000E+00	3.1324E-03	1.7043E-02	5.1787E-02	0.0000E+00	7.0223E-03
65	6.000E-01	0.0000E+00	3.2056E-03	2.1257E-02	5.0752E-02	0.0000E+00	6.8336E-03
66	6.600E-01	1.9323E-07	3.2832E-03	2.6528E-02	4.9841E-02	0.0000E+00	6.6832E-03
67	7.200E-01	2.8986E-06	3.3585E-03	3.2661E-02	4.8843E-02	0.0000E+00	6.5818E-03
68	7.800E-01	1.5661E-05	3.3746E-03	3.9266E-02	4.7514E-02	0.0000E+00	6.5071E-03
69	8.400E-01	6.6142E-05	2.2169E-03	4.7794E-02	4.4836E-02	0.0000E+00	6.4578E-03
70	9.200E-01	1.2649E-04	1.5900E-03	5.8195E-02	3.9872E-02	0.0000E+00	6.4400E-03
71	1.000E+00	4.7507E-04	1.3653E-03	7.7546E-02	3.1000E-02	0.0000E+00	6.3675E-03
72	1.200E+00	1.3397E-03	1.2528E-03	1.0591E-01	2.2000E-02	0.0000E+00	5.3650E-03
73	1.400E+00	2.8790E-03	1.2701E-03	1.3346E-01	1.7250E-02	0.0000E+00	4.2900E-03
74	1.600E+00	5.5374E-03	1.3530E-03	1.5895E-01	1.4000E-02	0.0000E+00	3.7125E-03
75	1.800E+00	1.6833E-02	1.2799E-03	1.8171E-01	1.1750E-02	0.0000E+00	3.3375E-03
76	2.000E+00	3.4659E-02	1.1650E-03	2.0568E-01	1.0190E-02	4.5627E-06	2.9850E-03
77	2.300E+00	6.0858E-02	9.7963E-04	2.2830E-01	8.5934E-03	2.6985E-05	2.6617E-03
78	2.600E+00	1.0624E-01	9.3978E-04	2.4453E-01	7.3000E-03	2.7197E-04	2.4250E-03
79	2.900E+00	1.7664E-01	9.0408E-04	2.5641E-01	6.1250E-03	1.9161E-03	2.1913E-03
80	3.300E+00	2.0612E-01	8.6934E-04	2.6349E-01	5.3000E-03	7.8766E-03	1.9500E-03
81	3.700E+00	2.7314E-01	8.3674E-04	2.6544E-01	4.5125E-03	1.9232E-02	1.7131E-03
82	4.100E+00	3.0799E-01	7.9224E-04	2.6420E-01	4.0000E-03	3.7202E-02	1.5450E-03
83	4.500E+00	3.6446E-01	7.4280E-04	2.6099E-01	3.5500E-03	6.2629E-02	1.3875E-03
84	5.000E+00	4.1781E-01	6.8479E-04	2.5676E-01	3.1000E-03	8.2816E-02	1.2375E-03
85	5.500E+00	4.5325E-01	6.2581E-04	2.5258E-01	2.7000E-03	1.0900E-01	1.1125E-03
86	6.000E+00	4.7619E-01	5.5346E-04	2.4914E-01	2.2900E-03	1.5813E-01	9.8875E-04
87	6.700E+00	4.8099E-01	4.7260E-04	2.4721E-01	1.8700E-03	2.0595E-01	8.6625E-04
88	7.400E+00	4.8208E-01	3.9198E-04	2.4582E-01	1.4288E-03	2.3413E-01	7.3813E-04
89	8.200E+00	4.8344E-01	3.2134E-04	2.3679E-01	1.1500E-03	2.5339E-01	6.7000E-04
90	9.000E+00	4.8084E-01	2.7027E-04	1.9918E-01	9.2501E-04	2.7294E-01	6.2500E-04
91	1.000E+01	4.7386E-01	2.4132E-04	1.3281E-01	7.7001E-04	2.9235E-01	6.3750E-04
92	1.100E+01	4.6280E-01	2.9059E-04	8.1568E-02	7.1000E-04	3.0281E-01	7.1250E-04
93	1.200E+01	4.3047E-01	4.8351E-04	5.5691E-02	6.5000E-04	2.9726E-01	8.0000E-04
94	1.300E+01	3.7927E-01	8.2254E-04	4.3526E-02	5.9000E-04	2.7461E-01	8.7500E-04

95	1.400E+01	3.0570E-01	1.1366E-03	3.7100E-02	5.3000E-04	2.4085E-01	8.7489E-04	
96	1.500E+01	2.4257E-01	1.2421E-03	3.3070E-02	4.8000E-04	2.0422E-01	7.5000E-04	
97	1.600E+01	1.9911E-01	1.1819E-03	3.0134E-02	4.4000E-04	1.7005E-01	5.5000E-04	
98	1.700E+01	1.6653E-01	1.0863E-03	2.7741E-02	4.0000E-04	1.4107E-01	3.7500E-04	
99	1.800E+01	1.4222E-01	1.0084E-03	2.5674E-02	3.6000E-04	1.1761E-01	2.8751E-04	
100	1.900E+01	1.2619E-01	9.5674E-04	2.3823E-02	3.2000E-04	9.8924E-02	2.6250E-04	
	2.000E+01							

DIFFERENTIAL FLUXES (input is normalized by a factor of 1.0500E+00)

		DIFFERENTIAL FLUX			STD. DEV. %			INTEGRAL	
GRP	ENERGY	NEW	OLD	RATIO	NEW	OLD	RATIO	FLUX > E	± %
1	1.0000E-10	2.5656E+19	9.4373E+19	0.272	25.41	55.24	0.460	3.7093E+14	5.75
2	1.0000E-09	3.1597E+20	9.0512E+20	0.349	15.42	46.49	0.332	3.7091E+14	5.75
3	1.0000E-08	7.8395E+20	1.9547E+21	0.401	8.33	41.21	0.202	3.6807E+14	5.85
4	2.3000E-08	8.8670E+20	2.0728E+21	0.428	4.36	38.80	0.112	3.5787E+14	6.17
5	5.0000E-08	6.7577E+20	1.4778E+21	0.457	6.27	37.09	0.169	3.3393E+14	6.79
6	7.6000E-08	3.8100E+20	7.7818E+20	0.490	10.55	35.95	0.294	3.1636E+14	7.16
7	1.1500E-07	1.6483E+20	3.1104E+20	0.530	14.70	34.89	0.421	3.0150E+14	7.37
8	1.7000E-07	6.6523E+19	1.1547E+20	0.576	18.27	33.87	0.539	2.9244E+14	7.46
9	2.5500E-07	3.3193E+19	5.3055E+19	0.626	21.14	32.87	0.643	2.8678E+14	7.47
10	3.8000E-07	2.1659E+19	3.2070E+19	0.675	23.35	31.94	0.731	2.8264E+14	7.47
11	5.5000E-07	1.4962E+19	2.0673E+19	0.724	24.88	31.01	0.802	2.7895E+14	7.44
12	8.4000E-07	9.9682E+18	1.2963E+19	0.769	25.79	30.05	0.858	2.7461E+14	7.39
13	1.2750E-06	6.6963E+18	8.2773E+18	0.809	26.23	29.15	0.900	2.7028E+14	7.33
14	1.9000E-06	4.6341E+18	5.4962E+18	0.843	26.32	28.31	0.930	2.6609E+14	7.27
15	2.8000E-06	3.1817E+18	3.6510E+18	0.871	26.10	27.48	0.950	2.6192E+14	7.20
16	4.2500E-06	2.1348E+18	2.3876E+18	0.894	25.68	26.66	0.963	2.5731E+14	7.12
17	6.3000E-06	1.4669E+18	1.6095E+18	0.911	25.15	25.91	0.971	2.5293E+14	7.05
18	9.2000E-06	1.0286E+18	1.1129E+18	0.924	24.54	25.19	0.974	2.4868E+14	6.99
19	1.3500E-05	6.8628E+17	7.3504E+17	0.934	23.82	24.43	0.975	2.4426E+14	6.93
20	2.1000E-05	4.6074E+17	4.9002E+17	0.940	23.10	23.72	0.974	2.3911E+14	6.87
21	3.0000E-05	3.2442E+17	3.4337E+17	0.945	22.39	23.06	0.971	2.3496E+14	6.84
22	4.5000E-05	2.1481E+17	2.2652E+17	0.948	21.63	22.36	0.967	2.3010E+14	6.81
23	6.9000E-05	1.4346E+17	1.5085E+17	0.951	20.90	21.71	0.963	2.2494E+14	6.80
24	1.0000E-04	1.0270E+17	1.0773E+17	0.953	20.27	21.18	0.957	2.2049E+14	6.80
25	1.3500E-04	7.9356E+16	8.3058E+16	0.955	19.75	20.77	0.951	2.1690E+14	6.82
26	1.7000E-04	6.2789E+16	6.5564E+16	0.958	19.27	20.40	0.945	2.1412E+14	6.84
27	2.2000E-04	4.9021E+16	5.1051E+16	0.960	18.78	20.03	0.938	2.1098E+14	6.86
28	2.8000E-04	3.8609E+16	4.0090E+16	0.963	18.32	19.67	0.931	2.0804E+14	6.88
29	3.6000E-04	3.0673E+16	3.1751E+16	0.966	17.89	19.33	0.926	2.0495E+14	6.90
30	4.5000E-04	2.4284E+16	2.5057E+16	0.969	17.50	19.00	0.921	2.0219E+14	6.93
31	5.7500E-04	1.8863E+16	1.9400E+16	0.972	17.11	18.64	0.918	1.9916E+14	6.96
32	7.6000E-04	1.4676E+16	1.5047E+16	0.975	16.78	18.29	0.917	1.9567E+14	6.99
33	9.6000E-04	1.1376E+16	1.1630E+16	0.978	16.49	17.95	0.919	1.9273E+14	7.02
34	1.2750E-03	8.8415E+15	9.0148E+15	0.981	16.25	17.61	0.922	1.8915E+14	7.05
35	1.6000E-03	7.1959E+15	7.3197E+15	0.983	16.08	17.33	0.928	1.8627E+14	7.08
36	2.0000E-03	5.6415E+15	5.7263E+15	0.985	15.89	17.00	0.935	1.8340E+14	7.11
37	2.7000E-03	4.3109E+15	4.3676E+15	0.987	15.71	16.67	0.942	1.7945E+14	7.14
38	3.4000E-03	3.3984E+15	3.4376E+15	0.989	15.55	16.37	0.950	1.7643E+14	7.17
39	4.5000E-03	2.7127E+15	2.7402E+15	0.990	15.40	16.08	0.958	1.7269E+14	7.20
40	5.5000E-03	2.1630E+15	2.1823E+15	0.991	15.26	15.81	0.965	1.6998E+14	7.22
41	7.2000E-03	1.6780E+15	1.6913E+15	0.992	15.07	15.52	0.971	1.6630E+14	7.24
42	9.2000E-03	1.3262E+15	1.3356E+15	0.993	14.98	15.34	0.976	1.6294E+14	7.26
43	1.2000E-02	1.0584E+15	1.0651E+15	0.994	15.00	15.29	0.981	1.5923E+14	7.28
44	1.5000E-02	8.5896E+14	8.6392E+14	0.994	15.06	15.29	0.985	1.5606E+14	7.29
45	1.9000E-02	6.8458E+14	6.8817E+14	0.995	15.10	15.29	0.988	1.5262E+14	7.30
46	2.5500E-02	5.5036E+14	5.5298E+14	0.995	15.14	15.29	0.990	1.4817E+14	7.29

47	3.2000E-02	4.5103E+14	4.5298E+14	0.996	15.17	15.29	0.992	1.4459E+14	7.29
48	4.0000E-02	3.6874E+14	3.7020E+14	0.996	15.19	15.29	0.993	1.4099E+14	7.28
49	5.2500E-02	3.0594E+14	3.0703E+14	0.996	15.20	15.29	0.994	1.3638E+14	7.25
50	6.6000E-02	2.4784E+14	2.4864E+14	0.997	15.21	15.29	0.995	1.3225E+14	7.23
51	8.8000E-02	2.0278E+14	2.0337E+14	0.997	15.22	15.29	0.995	1.2679E+14	7.19
52	1.1000E-01	1.7765E+14	1.7809E+14	0.998	15.22	15.29	0.996	1.2233E+14	7.15
53	1.3500E-01	1.5627E+14	1.5659E+14	0.998	15.22	15.29	0.996	1.1789E+14	7.12
54	1.6000E-01	1.3794E+14	1.3817E+14	0.998	15.22	15.29	0.995	1.1398E+14	7.08
55	1.9000E-01	1.2647E+14	1.2661E+14	0.999	15.21	15.29	0.995	1.0985E+14	7.03
56	2.2000E-01	1.1687E+14	1.1693E+14	0.999	15.20	15.29	0.994	1.0605E+14	6.99
57	2.5500E-01	1.0716E+14	1.0714E+14	1.000	15.17	15.29	0.992	1.0196E+14	6.93
58	2.9000E-01	9.9540E+13	9.9423E+13	1.001	15.14	15.29	0.990	9.8210E+13	6.87
59	3.2000E-01	9.2615E+13	9.2398E+13	1.002	15.08	15.29	0.986	9.5224E+13	6.82
60	3.6000E-01	8.6051E+13	8.5723E+13	1.004	15.01	15.29	0.981	9.1520E+13	6.74
61	4.0000E-01	8.0116E+13	7.9663E+13	1.006	14.90	15.29	0.974	8.8078E+13	6.67
62	4.5000E-01	7.2935E+13	7.2359E+13	1.008	14.75	15.29	0.964	8.4072E+13	6.57
63	5.0000E-01	6.4794E+13	6.4103E+13	1.011	14.54	15.29	0.951	8.0425E+13	6.48
64	5.5000E-01	5.7740E+13	5.6935E+13	1.014	14.27	15.29	0.933	7.7185E+13	6.39
65	6.0000E-01	5.4355E+13	5.3389E+13	1.018	13.92	15.29	0.910	7.4298E+13	6.30
66	6.6000E-01	5.3799E+13	5.2605E+13	1.023	13.48	15.29	0.882	7.1037E+13	6.19
67	7.2000E-01	5.2853E+13	5.1419E+13	1.028	12.95	15.29	0.847	6.7809E+13	6.08
68	7.8000E-01	4.9864E+13	4.8244E+13	1.034	12.33	15.29	0.807	6.4638E+13	5.95
69	8.4000E-01	4.5001E+13	4.3284E+13	1.040	11.63	15.29	0.761	6.1646E+13	5.83
70	9.2000E-01	4.0551E+13	3.8772E+13	1.046	10.86	15.29	0.710	5.8046E+13	5.67
71	1.0000E+00	3.7137E+13	3.5300E+13	1.052	10.06	15.29	0.658	5.4802E+13	5.51
72	1.2000E+00	3.3721E+13	3.1877E+13	1.058	9.24	15.29	0.604	4.7374E+13	5.15
73	1.4000E+00	3.0088E+13	2.8308E+13	1.063	8.45	15.29	0.552	4.0630E+13	4.82
74	1.6000E+00	2.6153E+13	2.4515E+13	1.067	7.71	15.29	0.504	3.4613E+13	4.55
75	1.8000E+00	2.2192E+13	2.0753E+13	1.069	7.06	15.29	0.461	2.9382E+13	4.32
76	2.0000E+00	1.7889E+13	1.6716E+13	1.070	6.50	15.29	0.425	2.4944E+13	4.12
77	2.3000E+00	1.3479E+13	1.2608E+13	1.069	6.06	15.29	0.396	1.9577E+13	3.87
78	2.6000E+00	1.0191E+13	9.5604E+12	1.066	5.69	15.29	0.372	1.5533E+13	3.67
79	2.9000E+00	7.5052E+12	7.0740E+12	1.061	5.39	15.29	0.352	1.2476E+13	3.52
80	3.3000E+00	5.4961E+12	5.2137E+12	1.054	5.10	15.29	0.334	9.4737E+12	3.40
81	3.7000E+00	4.2823E+12	4.0944E+12	1.046	4.81	15.29	0.314	7.2752E+12	3.39
82	4.1000E+00	3.4122E+12	3.2918E+12	1.037	4.51	15.29	0.295	5.5623E+12	3.52
83	4.5000E+00	2.5456E+12	2.4794E+12	1.027	4.26	15.29	0.279	4.1974E+12	3.79
84	5.0000E+00	1.7712E+12	1.7420E+12	1.017	4.16	15.29	0.272	2.9246E+12	4.34
85	5.5000E+00	1.2418E+12	1.2329E+12	1.007	4.35	15.29	0.285	2.0390E+12	5.06
86	6.0000E+00	8.0891E+11	8.1000E+11	0.999	4.92	15.29	0.321	1.4180E+12	5.82
87	6.7000E+00	4.8913E+11	4.9345E+11	0.991	5.81	15.29	0.380	8.5181E+11	6.89
88	7.4000E+00	2.8571E+11	2.8997E+11	0.985	6.92	15.29	0.453	5.0942E+11	7.96
89	8.2000E+00	1.5570E+11	1.5872E+11	0.981	8.15	15.29	0.533	2.8086E+11	9.11
90	9.0000E+00	8.2148E+10	8.3990E+10	0.978	9.38	15.29	0.613	1.5630E+11	10.11
91	1.0000E+01	3.7830E+10	3.8734E+10	0.977	10.55	15.29	0.690	7.4153E+10	11.20
92	1.1000E+01	1.7895E+10	1.8326E+10	0.976	11.60	15.29	0.758	3.6323E+10	12.13
93	1.2000E+01	8.9844E+09	9.1928E+09	0.977	12.50	15.29	0.818	1.8428E+10	12.90
94	1.3000E+01	4.7131E+09	4.8148E+09	0.979	13.25	15.29	0.866	9.4441E+09	13.51
95	1.4000E+01	2.5935E+09	2.6440E+09	0.981	13.84	15.29	0.905	4.7309E+09	13.97
96	1.5000E+01	1.3276E+09	1.3504E+09	0.983	14.29	15.29	0.935	2.1374E+09	14.34
97	1.6000E+01	5.2808E+08	5.3585E+08	0.985	14.62	15.29	0.956	8.0979E+08	14.63
98	1.7000E+01	1.8893E+08	1.9128E+08	0.988	14.85	15.29	0.971	2.8170E+08	14.84
99	1.8000E+01	7.2085E+07	7.2833E+07	0.990	15.01	15.29	0.981	9.2777E+07	15.00
100	1.9000E+01	2.0693E+07	2.0870E+07	0.991	15.11	15.29	0.988	2.0693E+07	15.11
	2.0000E+01								

INTEGRALS OF SPECTRA

OLD SPECTRUM	4.8244E+14	±	16.848 %
NEW SPECTRUM	3.7093E+14	±	5.746 %

NEW DIFFERENTIAL FLUXES

ENERGY	FLUX	STDEV	ENERGY	FLUX	STDEV
1.00000E-10	2.56564E+19	25.41	8.80000E-02	2.02785E+14	15.22
1.00000E-09	3.15974E+20	15.42	1.10000E-01	1.77648E+14	15.22
1.00000E-08	7.83952E+20	8.33	1.35000E-01	1.56266E+14	15.22
2.30000E-08	8.86699E+20	4.36	1.60000E-01	1.37943E+14	15.22
5.00000E-08	6.75772E+20	6.27	1.90000E-01	1.26470E+14	15.21
7.60000E-08	3.81001E+20	10.55	2.20000E-01	1.16871E+14	15.20
1.15000E-07	1.64826E+20	14.70	2.55000E-01	1.07164E+14	15.17
1.70000E-07	6.65232E+19	18.27	2.90000E-01	9.95396E+13	15.14
2.55000E-07	3.31930E+19	21.14	3.20000E-01	9.26148E+13	15.08
3.80000E-07	2.16594E+19	23.35	3.60000E-01	8.60511E+13	15.01
5.50000E-07	1.49622E+19	24.88	4.00000E-01	8.01155E+13	14.90
8.40000E-07	9.96822E+18	25.79	4.50000E-01	7.29352E+13	14.75
1.27500E-06	6.69634E+18	26.23	5.00000E-01	6.47937E+13	14.54
1.90000E-06	4.63405E+18	26.32	5.50000E-01	5.77400E+13	14.27
2.80000E-06	3.18173E+18	26.10	6.00000E-01	5.43554E+13	13.92
4.25000E-06	2.13476E+18	25.68	6.60000E-01	5.37995E+13	13.48
6.30000E-06	1.46689E+18	25.15	7.20000E-01	5.28531E+13	12.95
9.20000E-06	1.02863E+18	24.54	7.80000E-01	4.98637E+13	12.33
1.35000E-05	6.86278E+17	23.82	8.40000E-01	4.50007E+13	11.63
2.10000E-05	4.60739E+17	23.10	9.20000E-01	4.05513E+13	10.86
3.00000E-05	3.24421E+17	22.39	1.00000E+00	3.71374E+13	10.06
4.50000E-05	2.14812E+17	21.63	1.20000E+00	3.37209E+13	9.24
6.90000E-05	1.43462E+17	20.90	1.40000E+00	3.00883E+13	8.45
1.00000E-04	1.02700E+17	20.27	1.60000E+00	2.61532E+13	7.71
1.35000E-04	7.93556E+16	19.75	1.80000E+00	2.21924E+13	7.06
1.70000E-04	6.27887E+16	19.27	2.00000E+00	1.78887E+13	6.50
2.20000E-04	4.90212E+16	18.78	2.30000E+00	1.34792E+13	6.06
2.80000E-04	3.86090E+16	18.32	2.60000E+00	1.01913E+13	5.69
3.60000E-04	3.06732E+16	17.89	2.90000E+00	7.50518E+12	5.39
4.50000E-04	2.42841E+16	17.50	3.30000E+00	5.49611E+12	5.10
5.75000E-04	1.88627E+16	17.11	3.70000E+00	4.28232E+12	4.81
7.60000E-04	1.46757E+16	16.78	4.10000E+00	3.41225E+12	4.51
9.60000E-04	1.13760E+16	16.49	4.50000E+00	2.54564E+12	4.26
1.27500E-03	8.84149E+15	16.25	5.00000E+00	1.77125E+12	4.16
1.60000E-03	7.19592E+15	16.08	5.50000E+00	1.24184E+12	4.35
2.00000E-03	5.64149E+15	15.89	6.00000E+00	8.08908E+11	4.92
2.70000E-03	4.31093E+15	15.71	6.70000E+00	4.89131E+11	5.81
3.40000E-03	3.39837E+15	15.55	7.40000E+00	2.85705E+11	6.92
4.50000E-03	2.71269E+15	15.40	8.20000E+00	1.55695E+11	8.15
5.50000E-03	2.16297E+15	15.26	9.00000E+00	8.21485E+10	9.38
7.20000E-03	1.67802E+15	15.07	1.00000E+01	3.78299E+10	10.55
9.20000E-03	1.32617E+15	14.98	1.10000E+01	1.78948E+10	11.60
1.20000E-02	1.05839E+15	15.00	1.20000E+01	8.98436E+09	12.50
1.50000E-02	8.58956E+14	15.06	1.30000E+01	4.71314E+09	13.25
1.90000E-02	6.84582E+14	15.10	1.40000E+01	2.59350E+09	13.84
2.55000E-02	5.50356E+14	15.14	1.50000E+01	1.32765E+09	14.29
3.20000E-02	4.51026E+14	15.17	1.60000E+01	5.28082E+08	14.62
4.00000E-02	3.68742E+14	15.19	1.70000E+01	1.88928E+08	14.85
5.25000E-02	3.05938E+14	15.20	1.80000E+01	7.20845E+07	15.01
6.60000E-02	2.47842E+14	15.21	1.90000E+01	2.06927E+07	15.11
			2.00000E+01	----------	-----

SUMMARY OF BROAD-GROUP FLUXES, FLUENCES, AND UNCERTAINTIES

IRRAD TIME [S] = 1.19931840E+07 ACT NORM = 1.00000000E+00

ENERGY	FLUX	FLUENCE		STDEV %	
thermal	9.1979E+13	1.1031E+21	±	5.28	(1E-4 eV – 0.55 eV)
epithermal	1.5662E+14	1.8784E+21	±	12.01	(0.55 eV – 110 keV)
fast	1.2233E+14	1.4671E+21	±	7.15	(110 keV – 20 MeV)
fast	5.4802E+13	6.5725E+20	±	5.51	(1 MeV – 20 MeV)

MINI-SPECTRUM

ENERGY	FLUX	FLUENCE		STDEV %
1.0000E-10	9.1979E+13	1.1031E+21	±	5.28
5.5000E-07	5.8461E+13	7.0113E+20	±	24.52
1.0000E-04	9.8161E+13	1.1773E+21	±	12.42
1.1000E-01	4.1907E+13	5.0260E+20	±	16.78
5.0000E-01	2.5623E+13	3.0730E+20	±	16.56
1.0000E+00	2.9858E+13	3.5810E+20	±	9.51
2.0000E+00	2.2019E+13	2.6408E+20	±	4.63
5.0000E+00	2.8504E+12	3.4186E+19	±	4.45
1.0000E+01	7.2016E+10	8.6370E+17	±	11.52
1.5000E+01	2.1374E+09	2.5635E+16	±	14.34
2.0000E+01				
TOTAL	3.7093E+14	4.4487E+21	±	5.75

RELATIVE COVARIANCES (10×10)

1000	109	-192	-2	-1	0	6	5	-1	-3
1000	135	12	9	7	0	4	11	14	
1000	194	28	10	-4	9	25	32		
1000	276	32	-66	26	26	27			
1000	371	-88	34	60	36				
1000	341	-143	94	67					
1000	-330	-250	-87						
1000	356	89							
1000	777								
1000									

SPECTRAL-AVERAGED REACTION RATES (for all cross section library reactions)

REACTIONS	SIG-PHI	<SIG>	REACTIONS	SIG-PHI	<SIG>	REACTIONS	SIG-PHI	<SIG>
LI6(N,A)T	6.7504E-08	1.8198E-22	FE54(N,A)CR51	4.5592E-14	1.2291E-28	IN115(N,N')IN115M	1.3681E-11	3.6883E-26
B10(N,A)LI7	2.7520E-07	7.4192E-22	FE56(N,P)MN56	5.9167E-14	1.5951E-28	IN115(N,2N)IN114M	5.0732E-14	1.3677E-28
F19(N,2N)F18	4.9901E-16	1.3453E-30	FE58(N,G)FE59	1.0360E-10	2.7931E-25	IN115(N,G)IN116M	3.7682E-08	1.0159E-22
NA23(N,2N)NA22	2.5382E-16	6.8427E-31	CO59(N,2N)CO58	1.3116E-14	3.5359E-29	I127(N,2N)I126	6.9937E-14	1.8854E-28
NA23(N,G)NA24	3.8899E-11	1.0487E-25	CO59(N,G)CO60	3.4205E-09	9.2212E-24	LA139(N,G)LA140	7.3166E-10	1.9725E-24
MG24(N,P)NA24	8.4090E-14	2.2670E-28	CO59(N,A)MN56	8.5762E-15	2.3121E-29	PR141(N,2N)PR140	6.3099E-14	1.7011E-28
AL27(N,P)MG27	2.1929E-13	5.9119E-28	NI58(N,2N)NI57	2.7984E-16	7.5441E-31	TM169(N,2N)TM168	2.1288E-13	5.7391E-28
AL27(N,A)NA24	3.9423E-14	1.0628E-28	NI58(N,P)CO58	6.2278E-12	1.6789E-26	TA181(N,G)TA182	8.7205E-09	2.3510E-23
P31(N,P)SI31	1.6510E-12	4.4510E-27	NI60(N,P)CO60	1.0428E-13	2.8113E-28	W186(N,G)W187	8.6558E-09	2.3335E-23
S32(N,P)P32	3.6669E-12	9.8856E-27	CU63(N,2N)CU62	6.3594E-15	1.7144E-29	AU197(N,2N)AU196	1.9353E-13	5.2175E-28
TI46(N,2N)TI45	3.3875E-16	9.1324E-31	CU63(N,G)CU64	3.5662E-10	9.6140E-25	AU197(N,G)AU198	2.3310E-08	6.2843E-23
TI46(N,P)SC46	6.1751E-13	1.6647E-27	CU63(N,A)CO60	2.8723E-14	7.7433E-29	HG199(N,N')HG199M	1.6448E-11	4.4342E-26
TI47(N,P)SC47	1.0982E-12	2.9606E-27	CU65(N,2N)CU64	2.1163E-14	5.7053E-29	PB204(N,N')PB204M	9.6764E-13	2.6087E-27

TI47(N,X)SC46	5.7462E-16	1.5491E-30	ZN64(N,P)CU64	2.1679E-12	5.8444E-27	TH232(N,FISSION)	5.1414E-12	1.3861E-26
TI48(N,P)SC48	1.6496E-14	4.4472E-29	AS75(N,2N)AS74	1.9291E-14	5.2007E-29	TH232(N,G)TH233	1.4597E-09	3.9353E-24
TI48(N,X)SC47	1.1790E-16	3.1784E-31	Y89(N,2N)Y88	1.0688E-14	2.8813E-29	U235(N,FISSION)	4.0632E-08	1.0954E-22
TI49(N,X)SC48	7.1635E-17	1.9312E-31	ZR90(N,2N)ZR89	6.8371E-15	1.8432E-29	U238(N,FISSION)	2.1703E-11	5.8510E-26
V51(N,A)SC48	1.3594E-15	3.6647E-30	NB93(N,G)NB94	2.0564E-10	5.5439E-25	U238(N,G)U239	3.3795E-09	9.1108E-24
CR52(N,2N)CR51	2.9773E-15	8.0266E-30	NB93(N,N')NB93M	1.0767E-11	2.9028E-26	NP237(N,FISSION)	1.3043E-10	3.5164E-25
MN55(N,G)MN56	1.0343E-09	2.7883E-24	NB93(N,2N)NB92M	2.5090E-14	6.7641E-29	PU239(N,FISSION)	7.1643E-08	1.9314E-22
FE54(N,2N)FE53	9.1042E-17	2.4544E-31	RH103(N,N')RH103M	6.0374E-11	1.6276E-25	AM241(N,FISSION)	4.7841E-10	1.2898E-24
FE54(N,P)MN54	4.5556E-12	1.2281E-26	AG109(N,G)AG110M	1.0478E-09	2.8246E-24	SC45(N,G)SC46	1.9466E-09	5.2480E-24

INPUT FLUX REL. CORRELATION MATRIX (by row from diagonal)

1	1000	988	952	895	821	735	643	548	456	371	294	228	173	129	94	68	48	34	25	18
	14	12	10	9	9	8	8	8	8	9	9	9	9	9	9	10	10	10	10	10
	10	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11
	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11
	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11
2	1000	988	952	895	822	736	643	549	457	372	295	229	175	130	95	69	50	36	26	20
	16	13	12	11	10	10	10	10	10	10	11	11	11	11	11	12	12	12	12	12
	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13
	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13
	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	13	
3	1000	988	952	895	822	736	643	549	458	372	296	230	176	131	97	70	51	37	28	21
	17	15	13	12	12	12	12	12	12	12	12	12	13	13	13	13	14	14	14	14
	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14
	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14
	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14		
4	1000	988	952	896	822	736	644	549	458	373	297	231	176	132	97	71	52	38	28	22
	18	15	14	13	13	12	12	13	13	13	13	13	14	14	14	14	15	15	15	15
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	15	15	15	15	15	15	15	15	15	15	15	15	15	15	15	15	15			
5	1000	988	952	896	822	736	644	550	458	373	297	231	177	132	98	72	52	39	29	23
	19	16	15	14	13	13	13	13	14	14	14	14	15	15	15	15	16	16	16	16
	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16
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	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16				
6	1000	988	952	896	822	737	644	550	459	374	297	232	177	133	98	72	53	39	30	23
	19	17	15	14	14	14	14	14	14	14	15	15	15	16	16	16	16	16	16	16
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	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16					
7	1000	988	952	896	822	737	644	550	459	374	298	232	178	134	99	73	54	40	30	24
	20	17	16	15	15	15	15	15	15	15	15	16	16	16	17	17	17	17	17	17
	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17	17
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	17	17	17	17	17	17	17	17	17	17	17	17	17	17						
8	1000	988	952	896	822	737	644	550	459	374	298	233	178	134	100	74	54	41	31	25
	21	18	16	16	15	15	15	15	16	16	16	17	17	17	17	17	17	17	17	17
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	17	17	17	17	17	17	17	17	17	17	17	17	17							
9	1000	988	952	896	822	737	645	551	459	375	299	233	179	135	100	74	55	41	32	25
	21	19	17	16	16	16	16	16	16	17	17	17	18	18	18	18	18	18	18	18
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	18	18	18	18	18	18	18	18	18	18	18	18								
10	1000	988	952	896	822	737	645	551	460	375	299	234	179	135	101	75	56	42	32	26

	22	19	18	17	17	17	17	17	17	18	18	18	18	18	18	18	18	18	18	18
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	18	18	18	18	18	18	18	18	18	18	18									
11	1000	988	952	896	823	737	645	551	460	375	300	234	180	136	102	75	56	43	33	27
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	19	19	19	19	19	19	19	19	19	19										
12	1000	988	952	896	823	737	645	552	461	376	300	235	181	137	102	76	57	43	34	27
	23	21	19	19	18	18	19	19	19	19	20	20	20	20	20	20	20	20	20	20
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13	1000	988	952	896	823	738	646	552	461	376	301	236	181	137	103	77	58	44	35	28
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	21	21	21	21	21	21	21													
15	1000	988	952	896	823	738	646	553	462	377	302	237	182	139	104	78	59	46	36	30
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	21	21	21	21	21	21														
16	1000	988	952	896	823	738	646	553	462	378	303	237	183	139	105	79	60	46	37	31
	27	24	23	22	22	22	22	22	22	22	22	22	22	22	22	22	22	22	22	22
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	22	22	22	22	22															
17	1000	988	952	896	823	738	647	553	463	378	303	238	184	140	106	80	61	47	38	32
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	23	23	23	23																
18	1000	988	953	896	824	739	647	554	463	379	304	239	185	141	107	81	62	48	39	33
	29	26	25	24	24	24	24	23	23	23	23	23	23	23	23	23	23	23	23	23
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	23	23	23																	
19	1000	988	953	897	824	739	647	554	464	380	304	239	185	142	108	82	63	49	40	34
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	24	24																		
20	1000	988	953	897	824	739	648	555	464	380	305	240	186	143	108	83	64	50	41	35
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	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25
	25																			
21	1000	988	953	897	824	739	648	555	465	381	306	241	187	143	109	84	65	51	42	36
	32	30	28	27	26	26	26	26	26	26	26	26	26	26	26	26	26	26	26	26
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22	1000	988	953	897	824	740	648	555	465	381	306	242	188	144	110	85	66	52	43	37
	33	31	29	28	27	27	27	26	26	26	26	26	26	26	26	26	26	26	26	26
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23	1000	988	953	897	824	740	649	556	466	382	307	243	189	145	112	86	67	54	45	38
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	27	27	27	27	27	27	27	27	27	27	27	27	27	27	27	27	27	27		
24	1000	988	953	897	825	740	649	556	466	383	308	243	190	146	113	87	68	55	45	39
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	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28			
25	1000	988	953	897	825	740	649	557	467	383	309	244	191	147	113	88	69	56	46	40
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	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28	28			
26	1000	988	953	897	825	741	650	557	467	384	309	245	191	148	114	89	70	56	47	40
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27	1000	988	953	897	825	741	650	558	468	384	310	246	192	149	115	90	71	57	47	41
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29	1000	988	953	897	825	741	651	558	469	386	311	247	194	151	117	91	72	58	48	42
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	38	35	33	32	32	31	31	31	31	31	31	31	31	31	31	31	31	31	31	31
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31	1000	988	953	898	826	742	651	559	470	387	313	249	195	152	118	92	73	59	49	43
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32	1000	988	953	898	826	742	652	560	471	388	314	249	196	152	118	92	73	59	50	43
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34	1000	988	953	898	826	743	653	561	472	389	315	250	197	153	119	93	74	61	51	45
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	33	33	33	33	33	33	33													
35	1000	988	953	898	826	743	653	561	472	389	315	251	197	154	120	94	75	61	52	45
	41	38	36	35	35	34	34	34	34	34	34	34	34	34	34	34	34	34	34	34
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36	1000	988	953	898	827	743	653	562	473	390	315	251	198	154	120	95	76	62	52	46
	42	39	37	36	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35
	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35
	35	35	35	35	35															
37	1000	988	953	898	827	744	654	562	473	390	316	252	198	155	121	95	76	63	53	46
	42	39	38	37	36	36	36	35	35	35	35	35	35	35	35	35	35	35	35	35
	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35
	35	35	35	35																
38	1000	988	953	899	827	744	654	562	473	391	316	252	199	156	122	96	77	63	54	47
	43	40	38	37	37	36	36	36	36	36	36	36	36	36	36	36	36	36	36	36
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	36	36	36																	
39	1000	988	954	899	827	744	654	563	474	391	317	253	199	156	122	96	77	64	54	48
	43	41	39	38	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37
	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37
	37	37																		
40	1000	988	954	899	827	744	655	563	474	391	317	253	200	157	123	97	78	64	55	48
	44	41	40	39	38	38	37	37	37	37	37	37	37	37	37	37	37	37	37	37
	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37	37
	37																			
41	1000	988	954	899	828	745	655	563	475	392	318	254	201	157	123	98	79	65	56	49
	45	42	40	39	39	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38
42	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38	38
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43	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38		
44	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
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45	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38				
46	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38	38	38					
47	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38	38						
48	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38	38							
49	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38	38								
50	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38	38									
51	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38	38										
52	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38	38											
53	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50

	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38	38												
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	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38	38													
55	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38	38	38														
56	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
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57	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38	38																
58	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38	38																	
59	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38	38																		
60	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
	38																			
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	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38	38	38
62	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
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63	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38	38		
64	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38	38			
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	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38	38				
66	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38	38					
67	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38	38						
68	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38	38							
69	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39	39	38	38	38	38								
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	45	43	41	40	39	39	39	39	38	38	38									
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	45	43	41	40	39	39	39	39	38	38										
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	45	43	41	40	39	39	39	39	38											
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	45	43	41	40	39	39	39	39												
74	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39	39													
75	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39	39														
76	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40	39															
77	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41	40																

78	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43	41																	
79	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45	43																		
80	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	50
	45																			
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82	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66	56	
83	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79	66		
84	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98	79			
85	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124	98				
86	1000	988	954	899	828	745	655	564	475	392	318	254	201	158	124					
87	1000	988	954	899	828	745	655	564	475	392	318	254	201	158						
88	1000	988	954	899	828	745	655	564	475	392	318	254	201							
89	1000	988	954	899	828	745	655	564	475	392	318	254								
90	1000	988	954	899	828	745	655	564	475	392	318									
91	1000	988	954	899	828	745	655	564	475	392										
92	1000	988	954	899	828	745	655	564	475											
93	1000	988	954	899	828	745	655	564												
94	1000	988	954	899	828	745	655													
95	1000	988	954	899	828	745														
96	1000	988	954	899	828															
97	1000	988	954	899																
98	1000	988	954																	
99	1000	988																		
100	1000																			

OUTPUT FLUX REL. CORRELATION MATRIX (by row from diagonal)

1	1000	983	884	246	-692	-839	-839	-803	-754	-696	-635	-571	-509	-449	-395	-346	-305	-271	-244	-223
	-207	-195	-184	-175	-165	-153	-141	-127	-113	-97	-82	-68	-54	-42	-33	-24	-18	-14	-10	-8
	-7	-6	-6	-6	-6	-6	-6	-7	-7	-7	-7	-7	-8	-8	-8	-8	-8	-8	-8	-8
	-7	-7	-7	-7	-7	-6	-6	-5	-5	-5	-4	-3	-3	-2	-1	0	1	2	3	4
	4	4	4	3	1	0	-1	-2	-3	-4	-5	-5	-6	-6	-7	-7	-7	-8	-8	-8
2	1000	952	391	-614	-823	-856	-844	-812	-767	-715	-658	-599	-541	-487	-437	-395	-359	-331	-309	-292
	-278	-265	-253	-239	-224	-206	-186	-164	-142	-120	-98	-78	-61	-46	-34	-25	-18	-13	-10	-8
	-7	-6	-6	-6	-6	-7	-7	-7	-7	-8	-8	-8	-8	-8	-8	-8	-8	-8	-8	-8
	-8	-8	-7	-7	-7	-6	-6	-5	-5	-4	-3	-3	-1	0	0	1	3	4	5	5
	5	5	4	2	0	-1	-2	-3	-4	-5	-6	-6	-7	-7	-8	-8	-8	-9	-9	
3	1000	644	-384	-686	-778	-811	-815	-801	-776	-742	-703	-661	-620	-581	-547	-519	-496	-478	-463	-450
	-437	-420	-401	-376	-347	-314	-278	-240	-202	-166	-132	-102	-76	-56	-40	-28	-19	-14	-10	-8
	-7	-6	-6	-7	-7	-8	-8	-9	-9	-9	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
	-9	-9	-9	-8	-8	-7	-7	-6	-5	-4	-3	-1	0	1	3	4	6	7	8	8
	8	6	4	1	0	-2	-4	-5	-6	-7	-8	-8	-9	-10	-10	-10	-11	-11		
4	1000	445	68	-118	-241	-334	-410	-473	-525	-569	-606	-638	-665	-690	-712	-731	-747	-757	-761	-756
	-741	-715	-677	-628	-570	-506	-437	-368	-302	-240	-185	-139	-101	-71	-49	-33	-22	-15	-11	-9
	-8	-8	-8	-9	-10	-11	-12	-12	-13	-13	-14	-14	-14	-14	-14	-14	-14	-14	-14	-13
	-13	-12	-12	-11	-10	-9	-8	-7	-5	-3	-1	0	2	5	7	10	11	13	13	13
	11	7	3	0	-3	-5	-7	-9	-10	-11	-12	-13	-14	-14	-15	-16	-16			
5	1000	919	818	720	622	521	416	311	205	101	1	-91	-176	-252	-317	-370	-411	-440	-457	-461
	-453	-434	-407	-371	-330	-286	-241	-197	-157	-121	-90	-65	-45	-30	-19	-12	-7	-4	-2	-2
	-1	-2	-2	-2	-3	-3	-4	-4	-4	-5	-5	-5	-5	-5	-5	-5	-5	-5	-5	-4
	-4	-4	-4	-3	-3	-2	-2	-1	0	0	1	2	4	5	6	7	7	8	8	7
	5	3	1	0	-1	-2	-3	-3	-4	-4	-5	-5	-5	-6	-6	-6				
6	1000	977	930	868	793	708	614	513	410	306	206	112	28	-45	-107	-156	-193	-218	-232	-236
	-232	-220	-203	-182	-158	-133	-109	-86	-66	-49	-35	-23	-15	-9	-4	-1	0	0	1	1
	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	1	1	1	1	2	2	3	3	3	3	4	4	3	3

	2	2	1	1	0	0	0	0	0	0	0	0	0	0	0					
7	1000	986	952	900	833	753	662	564	463	361	264	174	94	25	-30	-74	-105	-126	-137	-141
	-137	-129	-117	-102	-86	-71	-56	-42	-31	-21	-14	-8	-4	-1	0	2	2	3	3	3
	3	3	3	3	3	3	3	2	2	2	2	2	2	2	2	2	2	2	2	2
	2	2	2	2	2	2	2	2	2	2	2	2	1	1	2	2	2	2	2	2
	2	2	2	2	2	2	2	2	2	2	2	2	2	2						
8	1000	989	958	909	844	765	675	577	477	377	282	195	120	56	5	-33	-60	-78	-87	-90
	-87	-80	-71	-61	-50	-39	-29	-21	-14	-8	-4	-1	1	2	3	4	4	5	5	5
	5	5	5	5	5	5	4	4	4	4	4	4	4	4	4	4	4	4	4	3
	3	3	3	3	3	3	2	2	2	1	1	1	1	0	0	1	1	2	2	2
	3	3	3	3	3	3	3	4	4	4	4	4	4							
9	1000	990	960	912	846	766	675	577	477	378	286	203	132	73	26	-8	-32	-47	-55	-58
	-55	-50	-44	-36	-28	-21	-15	-9	-5	-1	0	2	4	5	5	6	6	6	6	6
	6	6	6	6	6	6	6	6	6	6	6	6	6	6	5	5	5	5	5	5
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	4	4	4	4	5	5	5	5	5	6	6	6								
10	1000	990	960	911	844	763	671	572	472	375	286	206	138	83	40	8	-13	-26	-34	-36
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	8	8	8	8	8	8	8	8	8	7	7	7	7	7	7	7	6	6	6	6
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	5	5	6	6	6	6	7	7	7	7	8									
11	1000	990	959	909	840	757	664	565	466	371	284	207	143	91	50	21	1	-11	-18	-21
	-20	-18	-14	-10	-7	-3	0	1	3	5	6	7	7	8	8	8	9	9	9	9
	9	9	9	9	9	9	9	9	9	9	9	8	8	8	8	7	7	7	7	6
	6	5	5	4	3	2	1	0	0	0	-1	-1	0	0	1	2	4	4	5	6
	6	7	7	7	8	8	8	9	9	9										
12	1000	989	958	906	836	751	657	558	460	367	282	208	146	97	59	31	11	0	-7	-10
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	10	10	10	10	10	10	10	10	10	10	10	9	9	9	9	8	8	7	7	6
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	8	8	8	9	9	10	10	10	10											
13	1000	989	956	903	831	746	651	553	455	364	281	209	150	102	65	38	19	7	0	-2
	-3	-3	-1	0	1	3	5	6	7	8	9	10	10	10	11	11	11	11	11	12
	12	12	12	12	12	12	11	11	11	11	11	10	10	10	9	9	8	8	7	7
	6	5	4	2	1	0	0	-1	-2	-2	-1	0	1	3	4	6	7	7	8	8
	9	10	10	10	11	11	12	12												
14	1000	989	955	900	828	741	646	548	452	362	281	211	152	106	70	43	25	12	5	1
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	13	13	13	13	13	13	12	12	12	12	11	11	11	10	10	9	9	8	7	6
	5	4	3	1	0	0	-1	-2	-2	-1	0	1	3	5	6	7	8	9	9	10
	11	11	12	12	12	13	13													
15	1000	988	954	898	825	738	643	545	450	361	281	212	154	108	73	46	28	16	8	4
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	12	13	13	13	14	14														
16	1000	988	953	897	823	736	641	543	448	360	280	212	155	109	74	48	29	17	9	5
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	14	14	14	14	14	14	14	13	13	13	12	12	11	11	10	9	8	7	6	4
	3	1	0	-1	-2	-3	-3	-2	0	1	3	5	7	8	9	10	11	12	12	13
	13	14	14	15	15															
17	1000	988	952	896	821	734	639	542	447	359	280	211	155	109	74	47	29	17	9	5
	3	2	3	4	5	7	8	9	10	11	12	13	13	14	14	14	15	15	15	15
	15	15	15	15	15	14	14	14	13	13	12	12	11	10	10	9	8	6	5	3
	1	0	-1	-2	-3	-3	-2	-1	1	4	6	7	9	10	11	11	12	13	14	14
	15	15	16	16																
18	1000	988	952	895	820	733	638	541	446	358	278	210	153	107	72	45	27	15	7	3

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     17    18
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