Least-Squares Neutron Spectral Adjustment with STAYSL PNNL

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Abstract. The STAYSL PNNL computer code, a descendant of the STAY'SL code [1], performs neutron spectral adjustment of a starting neutron spectrum, applying a least squares method to determine adjustments based on saturated activation rates, neutron cross sections from evaluated nuclear data libraries, and all associated covariances. STAYSL PNNL is provided as part of a comprehensive suite of programs [2], where additional tools in the suite are used for assembling a set of nuclear data libraries and determining all required corrections to the measured data to determine saturated activation rates. Neutron cross section and covariance data are taken from the International Reactor Dosimetry File (IRDF-2002) [3], which was sponsored by the International Atomic Energy Agency (IAEA), though work is planned to update to data from the IAEA's International Reactor Dosimetry and Fusion File (IRDFF) [4]. The nuclear data and associated covariances are extracted from IRDF-2002 using the third-party NJOY99 computer code [5]. The NJpp translation code converts the extracted data into a library data array format suitable for use as input to STAYSL PNNL. The software suite also includes three utilities to calculate corrections to measured activation rates. Neutron self-shielding corrections are calculated as a function of neutron energy with the SHIELD code and are applied to the group cross sections prior to spectral adjustment, thus making the corrections independent of the neutron spectrum. The SigPhi Calculator is a Microsoft Excel spreadsheet used for calculating saturated activation rates from raw gamma activities by applying corrections for gamma self-absorption, neutron burn-up, and the irradiation history. Gamma self-absorption and neutron burn-up corrections are calculated (iteratively in the case of the burn-up) within the SigPhi Calculator spreadsheet. The irradiation history corrections are calculated using the BCF computer code and are inserted into the SigPhi Calculator workbook for use in correcting the measured activities. Output from the SigPhi Calculator is automatically produced, and consists of a portion of the STAYSL PNNL input file data that is required to run the spectral adjustment calculations. Within STAYSL PNNL, the least-squares process is performed in one step, without iteration, and provides rapid results on PC platforms. STAYSL PNNL creates multiple output files with tabulated results, data suitable for plotting, and data formatted for use in subsequent radiation damage calculations using the SPECTER computer code (which is not included in the STAYSL PNNL suite). All components of the software suite have undergone extensive testing and validation prior to release and test cases are provided with the package.

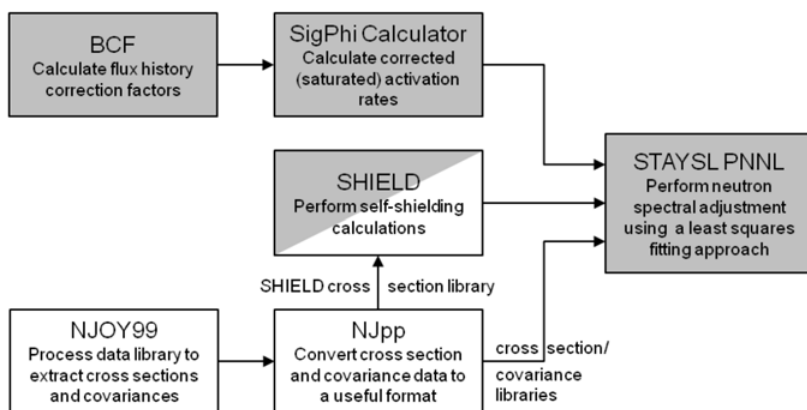[a] Corresponding author: `larry.greenwood@pnnl.gov`

Figure 1. Overview of software tools provided with STAYSL PNNL. Shaded boxes indicate tools that will be routinely used for each irradiation being evaluated, unshaded boxes indicate tools that will rarely be used, while the partially shaded box indicates a tool that may need to be applied depending on the scenario.

1. Background and Introduction

The STAY'SL computer code was originally written by Perey [1], who introduced the concept of using a generalized least-squares procedure for spectral adjustment, in contrast to the iterative "unfolding" procedures that had been developed previously. In the time since the release of STAY'SL, the first author made a number of improvements to the STAY'SL code by adding nuclear data libraries and making the code more user-friendly. The current incarnation, called STAYSL PNNL, includes major improvements to the code and bundles the main code with a number of utility programs in a comprehensive package that addresses all steps for applying nuclear data, covariances, and corrections to obtain an adjusted neutron spectrum. The software suite consists of the STAYSL PNNL, SHIELD, BCF, and NJpp Fortran codes and the SigPhi Calculator spreadsheet tool. In addition, the third-party NJOY99 Fortran code [5] is used for extraction of nuclear data and associated covariances from standard evaluated nuclear data libraries. After providing an overview of the software components and the work flow, the function of each of the STAYSL PNNL software suite programs is described in separate sections below, followed by examples of a typical spectral adjustment.

Figure 1 provides a general overview of the main steps that are required for neutron spectral adjustment. Processing of nuclear data using NJOY99 and NJpp (the unshaded boxes) is not required because the distributed code package already includes the required cross section and covariance libraries. The SigPhi Calculator spreadsheet tool facilitates making all known corrections to measured activation data to obtain saturated activation rates. The BCF code corrects for decay during irradiation for very complicated irradiation histories and the output is used by the SigPhi Calculator. The SHIELD code produces shielded cross sections for user-specified wire or foil fluence monitors prior to spectral adjustment. The STAYSL PNNL user manual [2] provides comprehensive documentation for all of the computer codes that are briefly described in the rest of this paper.

2. Nuclear Cross Sections and Covariances

Nuclear activation cross sections and associated covariances have been adopted from the International Reactor Dosimetry File of 2002 (IRDF-2002) [3] developed by the Nuclear Data Section of the International Atomic Energy Agency (IAEA; Vienna, Austria). The NJOY99 [5] and NJpp codes are used to assemble cross section and covariance input data libraries for both STAYSL PNNL and for neutron self-shielding and cover reactions, as discussed later. NJOY99 is not included with the STAYSL
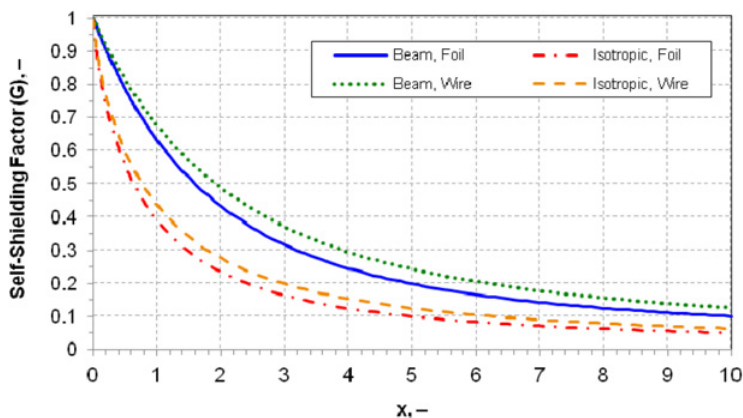
Figure 2. Plot of the neutron self-shielding factor as a function of the parameter x, representing the sample device dimensions and nuclear properties, for the four combinations of neutron environment (beam or isotropic) and sample device type (foil or wire). The parameter x is calculated as the thickness of the foil (or radius of the wire) times the atom density times the group neutron cross section.

PNNL software suite distribution package; however, it is not required unless the user wants to modify the currently existing libraries that are included with STAYSL PNNL. The current distribution package includes cross section and covariance libraries using a 100-group energy structure from 1.E-10 to 20 MeV. The distribution package also includes examples of NJOY99 input files that were used to generate the cross section and covariance libraries, in case users have access to NJOY99 and wish to use alternate group structures. The NJpp code was developed to read NJOY99 output files and reformat them into nuclear data libraries for subsequent use by STAYSL PNNL and SHIELD (as discussed later). Future work is planned to update the nuclear data libraries with the IRDFF (International Reactor Dosimetry and Fusion File), recently released by the IAEA [4].

3. Neutron Self-shielding Corrections with SHIELD

The SHIELD code calculates energy-dependent neutron self-shielding cross section correction factors that are used, prior to neutron spectral adjustment, to shield the neutron activation cross sections used by the STAYSL PNNL code. 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 (i.e., beam vs. isotropic neutron field). 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. The self-shielding correction factors are contained in a library used as input to STAYSL PNNL, so a user could simply run SHIELD once with all possible relevant monitor sample/flux environment conditions or could run SHIELD for every new scenario. SHIELD requires a library of cross sections, similar to 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 1.0E-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 equations used for calculating the very fine group shielding factors for each reaction are taken from an IAEA report [6] and are documented in the STAYSL PNNL user manual [2]. Figure 2 shows the neutron shielding factor for both wires and foils and for isotropic and beam neutron fluxes as a function of sample device dimensions and nuclear properties (i.e., thickness of the foil or radius of the wire times the atom density times the group neutron

cross section). These corrections are applied to the very fine energy grid used by SHIELD and then collapsed to the much coarser energy grid used for spectral adjustment.

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 neutron mean free path lengths), then neutron transport codes (for example, MCNP [7]) are required to correctly account for neutron self-shielding effects.

4. Irradiation History Corrections with BCF

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. 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 (beam correction factor) 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. Options are provided such that the user may input any combination of differential or integral reactor power, neutron flux or fluence, or accelerator beam current or charge. Corrections are determined using Eq. (1).

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

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 and XPROD is the integral of the flux-time product.

The output of the BCF computer code is copied to the SigPhi Calculator Excel spreadsheet such that the irradiation histories are automatically applied using a lookup table.

5. SigPhi Calculator

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" ($\sigma \bullet \phi$) 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 (i.e., burn-up of isotopes due to the neutron irradiation). The SigPhi Calculator applies the output from the BCF code to account for the production and decay over the timeframe of sample irradiation. 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, sample geometry (wire or foil), and sample thickness, while linear mass attenuation coefficients are taken from the XCOM database [8]. Neutron burn-up is calculated in the SigPhi Calculator based on irradiation event, reaction, and activation product isotope information. 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. The Excel spreadsheet comes with a number of worksheets containing all the data required to correct for nuclear decay, atomic weights, isotopic abundances, gamma self-absorption, and neutron burn-up. The user copies the output of the BCF computer code to one of the worksheets such that the spreadsheet will automatically access the appropriate irradiation history corrections as well as all of the other data from the various spreadsheet tabs.

Neutron burn-up corrections for non-threshold reactions are performed using an iterative technique. The uncorrected reaction rate for a given reaction is taken as the first approximation to determine the correction. This process is then iterated until the process converges at the appropriate value. The burn-up of the activation product isotope is included with each iteration by calculating the ratio of the burn-up rate for the product isotope to that of the target (starting) isotope (which is typically the best known). In cases where the nuclear burn-up depends on additional reactions (besides the reaction of interest), the total burn-up reaction rate is also determined by the ratio of the reactions. The ratios are approximated using the thermal neutron cross section and resonance integral in a process using the ratio of the epithermal to thermal neutron flux to provide the best fit to all of the measured reactions simultaneously (or as supplied by the user). Once burn-up corrections have been determined for the non-threshold reactions, the derived thermal and epithermal neutron fluxes are used to calculate burn-up corrections for the threshold nuclear reaction products. The iterative process will converge except in cases of very high burn-up where the solution is no longer unique because the quantity of product has begun to decline. In such cases, the user must determine the appropriate corrections by other means.

The primary output of the SigPhi Calculator is the saturated reaction rates with all required corrections applied. The user can have the SigPhi Calculator generate a block of text properly formatted for use as input to STAYSL PNNL and incorporating the resultant saturated reaction rates (as well as placeholders for additional inputs such as the initial neutron spectrum). The Sig-Phi Calculator will also provide a rough estimate of the thermal, epithermal, and fast neutron fluences. This is simply for the convenience of the user and provides a rapid way to check for data consistency. The thermal/epithermal fluences are determined by simultaneously fitting non-threshold data to the thermal neutron cross section

and resonance integrals. Because the neutron spectrum has not yet been determined, fast neutron fluences can be estimated using fission spectral-averaged cross sections as a first approximation. The user can choose how to normalize the neutron flux to any specified power level, such as time average or full reactor power. The neutron fluence values are, of course, invariant and neutron flux values are only provided for convenience of the user. Options selected in the SigPhi Calculator will be subsequently used in STAYSL PNNL (but may also be changed later, if so desired).

6. STAYSL PNNL Neutron Spectral Adjustment

Given a set of neutron activation rates measured in a nuclear fission reactor or 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 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 being a calculated result from a numerical code such as MCNP versus a generic "standard" spectrum). Covariances must be specified by the user for all input quantities. The output of STAYSL PNNL provides the adjusted neutron spectrum and a brief summary of broader group fluxes with 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. The code may also be used simply to calculate reaction rates for all of the reactions in the nuclear data library without doing any spectral adjustment.

There are many input options available with STAYSL PNNL to accommodate most reactor dosimetry applications. The saturated reaction rate values are normally output directly into a starting input file from the SigPhi Calculator spreadsheet. The user can add thermal neutron cover reactions (boron, cadmium, gadolinium, or gold) as well as neutron self-shielding (by referencing previously calculated factors that were added as output from the SHIELD code). The calculated input neutron spectrum is then specified with options for adding a thermal Maxwellian and a 1/E flux spectrum at thermal and epithermal neutron energies, respectively, in cases where those parts of the neutron spectrum are neither well-known nor previously calculated. Variances and covariances must be specified for all of the input data. This can be done by entering the covariance matrices directly or by using optional methods also provided in the code, such as constant covariance values between different measured reaction rates and Gaussian smoothing functions for calculated neutron spectra.

The main output from STAYSL PNNL lists all the details of the spectral adjustment including all the input data and options followed by calculated reaction rates and a neutron flux listing, showing values both before and after adjustment along with uncertainties and integral flux values. Files are also provided for plotting and for direct input into the SPECTER computer code [9], used for radiation damage calculations.

7. Example Application

An example of a spectral adjustment is shown in Figs. 3 through 5. In this case, the calculated neutron spectrum (Fig. 3) agrees well with the threshold reaction rates but the thermal neutron spectrum is about a factor of two higher than indicated by the measured non-threshold reaction rates. The spectral adjustment is thus very small in the fast energy region but reduces the thermal neutron flux spectrum to provide a very good fit to the data.

Figures 4 and 5 show portions of the main output file produced by STAYSL PNNL. Figure 4 shows the calculated reaction rates both before and after adjustment of the neutron spectrum.
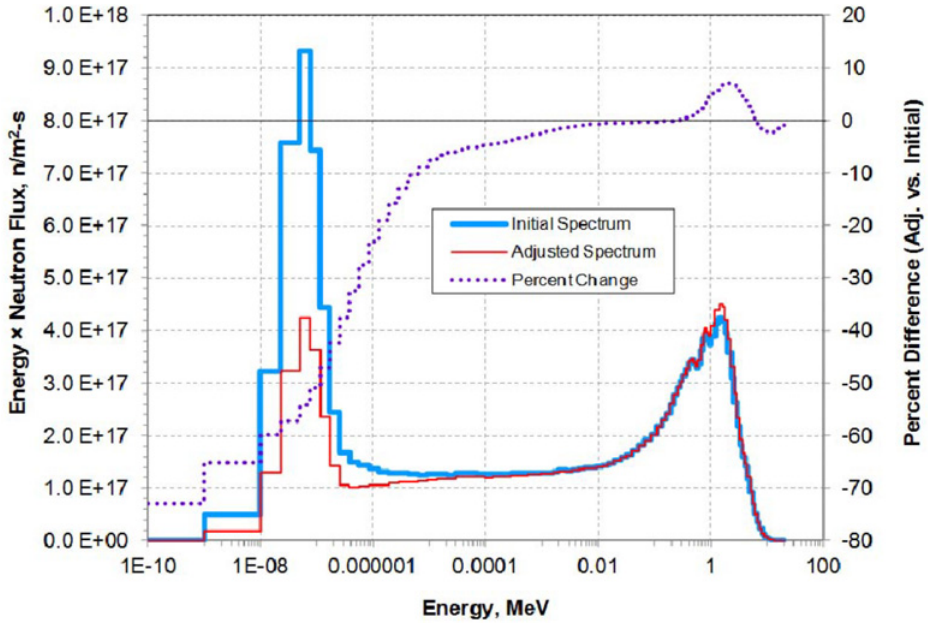
Figure 3. Neutron spectral adjustment for a typical research reactor using STAYSL PNNL. The plot shows the initial flux along with the adjusted spectrum and the percent difference (using the right axis) between the two.

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

STAYSL PNNL, version 1.0.2, 2013-Jan-07

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
```

Figure 4. Top portion of the main STAYSL PNNL output file. This portion of the output shows adjustment parameter settings and the Dosimetry Activities table, which lists measured data (after corrections) as well as the reaction rates for the unadjusted and the adjusted fluxes for each monitor sample reaction.

```
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
  .     .          .           .          .       .      .      .       .         .
  .     .          .           .          .       .      .      .       .         .
  .     .          .           .          .       .      .      .       .         .


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

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  ±   6.10     (1E-4 eV — 0.55 eV)
   epithermal  1.5662E+14  1.8784E+21  ±  11.30     (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)

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

      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
   B10(N,A)LI7       2.7520E-07  7.4192E-22   FE56(N,P)MN56     5.9167E-14  1.5951E-28
```

Figure 5. Portion of the main STAYSL PNNL output file showing the first few rows of the Differential Fluxes table, the summary of broad-group flux/fluences, and the first couple of rows of the Spectral-Averaged Reaction Rates table.

Whereas the initial neutron spectrum shows large disagreements with the measurements, the adjusted neutron spectrum agrees with all measurements within 6% and a normalized chi-square value (i.e., chi-square per degree of freedom, denoted as NORM CHI^2 in Fig. 4) that is less than 1. Figure 5 shows the first few rows of the numerical group flux adjustments (also depicted in Fig. 3) as well as a brief summary of broad neutron fluence values (with their uncertainties) and a the first few rows of a table of spectral-averaged reaction rates.

References

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