Release Notes for the STAYSL PNNL Suite v. 1.2.0 (2015-Aug-05)

The User Guide for the STAYSL PNNL Suite of Software Tools [Greenwood and Johnson, 2013] has not yet been updated to reflect the changes incorporated into version 1.2.0 of the STAYSL PNNL Suite of computer software (dated August 5, 2015). However, Figure 2 from the User Guide, has been updated and is attached here (Attachment A). Otherwise, these Release Notes serve, in the interim, to describe the changes to the STAYSL PNNL software since the previous full release on April 12, 2013. The user is encouraged to read this file before attempting to use the software because there are several notable changes.

Along with a number of minor improvements, two main aspects of functionality were implemented in this version 1.2.0 release: incorporation of cross sections and covariances from the International Reactor Dosimetry and Fusion File (IRDFF) version 1.05 data library and extension of the energy range to 60 MeV. The IRDFF library replaces the IRDF-2002 library (though with only a couple of exceptions, the IRDF-2002 library can still be applied, if the user desires) and includes data for updated evaluations and 12 new reactions. The user can now also work with an energy grid extending up to 60 MeV for high energy applications. Another significant change involves streamlining the way in which energy grid structure information is specified, making files more consistent and making the use of other energy grids easier.

Except for the BCF code (which has not been modified for this release), changes to each code are described below. The user is encouraged to report any software issues, errors, or concerns to the developers.

NJOY

NJOY itself has not been modified for this release (indeed, NJOY99 is a third-party software and is not specifically included with the STAYSL PNNL package; more information is available at http://t2.lanl.gov/codes/njoy99/). However, this STAYSL PNNL distribution includes updated NJOY output based on IRDFF v. 1.05. The IAEA Nuclear Data Service produced the International Reactor Dosimetry and Fusion File (IRDFF) as an updated and expanded successor to the IRDF-2002 nuclear data library. The latest version of IRDFF is 1.05, released on 2014-Oct-09 (https://www-nds.iaea.org/IRDFF/). IRDFF includes new data evaluations as well as new reactions (listed below in the NJpp section) and data for energies up to 60 MeV.

In addition to the default STAYSL PNNL 140-group energy grid structure, NJOY input files and the data output extracted from IRDFF are provided in the STAYSL PNNL distribution for five additional energy grid structures: 69-group (WIMS/EPRI-CPM), 129-group (for 14 MeV source), 175-group (VITAMIN-J), and 640-/725-group (SAND IIa). Energy structures are also included in separate files for user convenience. The previous NJOY input files for IRDF-2002 and the associated extracted output ("output_xsect_covar.dat" and "output_xsect_shield.dat") are still included for completeness.

Note that the NJOY input file "in_xsect_shield_irdff_14468.dat" for producing cross section data on a fine energy grid structure that can be used with SHIELD has been updated from the previous 14014-group structure. The energy range has been extended from 20 MeV to 60 MeV in 0.2 MeV steps. In addition, energy grid boundaries were added to the structure to accommodate all 6 of the abovementioned energy grid structures.

NJpp

NJpp was updated to include 12 new reactions in IRDFF (SI28P, MN552, CO593, CO59P, ZN67P, MO92P, IN113N, IN113G, TM1693, BI2093, U235G, and U2382). Note that the IRDFF v. 1.05 update of Table 4 from the INDC(NDS)-0616 document [Zsolnay et al., 2012] includes some additional items and variations that are not adopted for the PNNL STAYSL Suite. The IRDFF reaction SI29D is not included because there is no cross section data in the IRDFF library. While the reactions IN113(N,G)IN114, IN113(N,G)IN114G, and IN113(N,G)IN114M (with reaction codes of IN113G, IN113GG, and IN113GM, respectively) are included in IRDFF v. 1.05, the STAYSL PNNL Suite only recognizes the IN113(N,G)IN114M reaction because it alone has a half-life suitable for dosimetry measurements. Further, the short reaction name IN113G continues to be used to represent the IN113(N,G)IN114M reaction in the STAYSL PNNL Suite (in contrast to the abovementioned short reaction names found in IRDFF). In addition, IRDFF v. 1.05 shows a change in the reaction code for the IN115(N,2N)IN114m reaction to IN1152M; but the STAYSL PNNL Suite continues to use the short reaction name of IN1152.

An additional data item, "ZAM," was included in NJpp (and the "Reaction_Data" worksheet of the SigPhi Calculator) to distinguish reactions for cases where the MAT, MF, and MT numbers were insufficient to make the distinction (e.g., for "n,g" reactions of Niobium and Indium). NJpp also includes the IRDFF change in MAT number to 2125 for the Sc-45 (n,g) reaction (from the value of 2126 that was used in IRDF-2002).

The default behavior with respect to file names was altered. NJpp will now automatically append either "_covar" or "_xsect" to the root input file name to arrive at the output file name, depending on the user-selected mode of operation (covariances or cross sections). Thus, a NJpp input file name of "o.dat" (representing the file produced by NJOY) will result in a primary NJpp output file named "o_covar.out" when operated in covariance mode and named "o_xsect.out" when operated in cross section mode.

A couple of default values for NJpp run parameters have been altered to accommodate the new reactions and the expanded energy grid. Defaults are now 140 energy groups (formerly 100) and 80 materials maximum (formerly 70).

NJpp was updated to be consistent with changes to SHIELD and STAYSL PNNL. When processing covariance data, NJpp now allows up to 800 energy groups, versus the previous constraint of 700 energy groups. The output file generated by NJpp for cross section data now lists the number of energy groups on the first line instead of the number of energy group boundaries. This latter change makes the STAYSL PNNL suite consistent in using the number of energy groups throughout all codes (versus the previous mixture of number of energy groups and number of boundaries).

Note that, if you use an energy grid structure other than the default 140-group energy grid structure used by STAYSL PNNL, you may end up with output from NJOY/NJpp that does not have all of the reactions because the "threshold is above highest energy bound" of the energy grid. This issue was encountered for the WIMS (69-group) and the 14 MeV (129-group) energy grid structures (but not the 140-, 175-, 640-, or 725-energy group structures). This issue would impact which reactions you can use with certain energy grids when running STAYSL PNNL.

When NJpp is used to process NJOY output to obtain covariances for a large energy grid, some of the default NJpp run parameters may need to be altered to avoid memory problems (depending on the capabilities of your computer). For example, on the developer's system the 725-group energy grid required that the maximum number of reactions per material and the maximum number of materials be set to values of 6, and 54, respectively. This avoided excessive memory usage and still captured all of the reactions.

As discussed in the User Guide, the fine energy grid NJpp output for use with SHIELD must be manually edited to remove the data for the IN113N, IN115N, and IN1152 reactions (to give the "shld_xsect.out" file) because these reactions are threshold reactions.

For completeness…A feature unrelated to application of STAYSL PNNL was fixed in version 1.2.0 to provide proper header information for each block of reaction data when outputting covariance cross correlations.

SHIELD

The input file format has been revised to be more user-friendly, though backwards compatibility is maintained by still accepting the older input file format. The new format uses one line per monitor sample configuration and provides a comment field for user annotations.

In the original input file format, there are two lines (records) per monitor sample type:
```
<THK><ATN>                      (free format)
<sNameA><sWFvar><sTYP>          (A6,2X,A4,1X,A3 format)
```

In the new input file format, there is one line per monitor sample type:
```
<sNameA><sWFvar><sTYP><THK><ATN><sCmt> (A6,2X,A4,2X,A3,1X,*,*,A50 format
                                       [i.e., THK and ATN are free format])
```

Requirements for the neutron cross section data library input file name were changed to mesh with the above-discussed revisions to NJpp. The cross section library for SHIELD must now be named "shld_xsect.out" (instead of "shldxsect.out"). Similarly, SHIELD now expects that the number of energy groups (not number of boundaries) is specified in the cross section data file produced by NJpp, consistent with changes to NJpp.

The "shldengrp.dat" file is now an optional file, and the user can now set the name of this energy grid file to any valid file name. The user will be interactively asked for either the number of energy groups (with 69, 129, 140, 175, 640, or 725 being the only allowed options) or the name of an energy grid structure file. If a valid number is supplied, then SHIELD uses the internally defined list of energy grid boundaries (corresponding to the energy grid structures included in the NJOY directory, as mentioned above). Otherwise, SHIELD expects to open a file containing a header line (I10 format) with the number of energy groups and a record containing an array of energy grid boundaries (7E11.4 format). For consistency between codes, the energy grid boundaries in the file must be in units of eV, in contrast to the MeV units previously required in the "shldengrp.dat" file. User-supplied energy grids are converted internally to units of MeV. It is also possible to specify the run parameters file name and the energy grid options as command line arguments.

The output format of the SHIELD primary output file (*.out) was slightly altered to report the THK value in ES10.3 format instead of E10.3 format.

BCF

No changes were made to the BCF code.

SigPhi Calculator

The 12 new reactions (discussed above in the NJpp section) were added to the "Reaction_Data" worksheet. XCOM data for total photon absorption (including coherent scattering) was added to the "MassAttenuationCoeff" worksheet to expand the energy range to 60 MeV and to include data for Si, Mo, and Bi, which are needed for new reactions.

The σ and resonance integral values for four product isotopes involved in existing reactions were updated to use data from the Chart of the Nuclides [KAPL, 2010] rather than make estimates because Holden [2003] lacked data. One of the new reactions also uses data from the Chart of the Nuclides. Otherwise the new reactions use Holden [2003] or estimate values for product isotopes based on values for the target isotope. The values taken from the Chart of the Nuclides are listed in the table below.

Product Isotope	σ (barn/atom)	R.I. (barn/atom)
41-Nb-93m	0.9	6.2
45-Rh-103m	11	80
49-In-113m (new reaction)	5	220
49-In-115m	87	2600
53-I-126	5960	40600

Logic was added to the Gamma Self-Absorption calculation (column Q on the "SigPhi_Calculations" worksheet) to avoid a divide by zero error when the user selects a "Foil" sample type with a thickness of 0.0 (i.e., to represent a material deposited in a thin film on an X-ray mount, where gamma self-absorption is negligible). This makes the calculation consistent with the preferred approach described in the User Guide (and is more intuitive than using a sample type of "Wire").

Several items related to the "Export Sample Results for STAYSL PNNL" were updated. The default value for KG was changed to 140 to match the expanded energy grid. The default value used for FS was changed to 0.001 (instead of 0.03). Also, the sample name/ID is now automatically included as part of the "title" line in the exported data.

STAYSL PNNL

The expansion of the energy grid to 60 MeV means that older STAYSL PNNL input files will need to be updated to set KG to 140 and possibly to add an energy grid for the flux spectrum. A message about an error when reading FIN likely indicates that the flux spectrum energy groups do not match the 140-group energy grid and that the flux spectrum energy grid must be specified explicitly in the STAYSL PNNL input file (in record 18a or 18b). Alternately, the data for the flux spectrum could be expanded to the 140-group energy grid. Also, consistent with the constraints of NJpp, STAYSL PNNL now allows energy grids of up to 800 energy groups.

Several changes related to normalization/input parameters have been implemented. The display format of the RENORM value in the primary output file was altered to handle large numbers. However, the recommendation is that users put large normalization factors in TNORM and leave

AK1 for small normalization adjustments (small positive values). Negative values are no longer allowed for the AK1 parameter. The user can set AK1 to zero to indicate that STAYSL PNNL should use automated normalization (formerly referred to as "free-floating normalization"). The output for the SPE file when IPNT = 3, now shows reaction rates after corrections for TNORM, covers, self-shielding, and AK1 normalization (previously, the reaction rates had not included the AK1 normalization). In the case where $ACNM \neq 1.0$, the extra table of data printed in the primary output file between the scenario heading and the covariance parameters has been eliminated.

The approach to file names for data library files has been altered. STAYSL PNNL will now obtain the number of energy groups (KG) from the run input parameters file and will look for library files having names in the format of "xsectlib*nnn.dat", "covarlib*nnn.dat", and "sshldlib*nnn.dat", where nnn is the number of energy groups and the asterisk represents a wildcard indicating any number of other characters. If multiple files are found that match the pattern, STAYSL PNNL will use the first file whose energy group specification matches KG. If a file with a name in the above format is not found in the working directory, then STAYSL PNNL will attempt to use the generic file names of "xsectlib.dat", "covarlib.dat", and "sshldlib.dat". In all cases, the number of energy groups specified in the data library file must equal KG.

All library files (and the run parameters input file) must specify the energy grid size in terms of the number of energy groups, not the number of energy grid boundaries. Previously, input files/libraries used a mix of either number of groups or number of boundaries. NJpp has been altered to facilitate this change, as discussed above.

Activity values reported in the "DOSIMETRY ACTIVITIES" table of the STAYSL PNNL primary output file are now shown in units consistent with the input and the "SPECTRAL-AVERAGED REACTION RATES" table of the output. Previously, the units for these two output tables differed by a factor of 1×10^{24} barn/cm².

Changes were made to how the "DIFFERENTIAL FLUXES" table of the primary output file is written. The original output would end if all fluxes above a certain point in the energy grid were zero, but the ending boundary was still displayed as 20 MeV. For example:

```
96  1.5000E+01  ...
97  1.6000E+01  ...
    2.0000E+01
```

Here, the last two rows could be misinterpreted as a span from 16 MeV to 20 MeV, when really the span was from 16 to 17 MeV. The final row of the table will now show the actual upper boundary of the last displayed energy group.

Changes were implemented for the "SUMMARY OF BROAD-GROUP FLUXES, FLUENCES, AND UNCERTAINTIES" table in the STAYSL PNNL primary output file. A "high" category was added to show the flux, fluence, and standard deviation for the energy range from 20 to 60 MeV. The groups now dynamically select the energy grid boundary and show appropriate labeling. Boundaries for thermal, epithermal, fast, and high neutron energies are nominally defined as 1E-10, 5.5E-7, 0.11, 1.0, 20.0, and 60.0 MeV. The nearest energy grid boundary will

be used to make these general categories. The example output below illustrates the variations resulting from the use of the 175-group VITAMIN-J energy grid structure:

```
    ENERGY      FLUX       FLUENCE      STDEV %
  thermal    5.5965E+04  2.1479E+09  ± 182.59     (0.010 meV — 0.532  eV)
 epithermal  1.7842E+06  6.8474E+10  ±  28.08     (0.532  eV — 111.1 keV)
    fast     5.0295E+08  1.9303E+13  ±   1.19     (111.1 keV —  19.6 MeV)
    fast     4.9529E+08  1.9009E+13  ±   1.17     (  1.0 MeV —  19.6 MeV)
 key "high" energy not found in energy boundary list
```

The mini-spectrum definition continues to have ten bins, but the user will need to add more groups (to get to 140 groups total) or they will get a warning message (which is okay, but lumps more into the last bin). For mini-spectrum results in the primary output file, logic has been added to STAYSL PNNL to report flux, fluence, and standard deviation results as 0.0 when there is no flux in any of the energy groups within a particular mini-spectrum bin, which is more meaningful than the flux value of 1.0 previously used to avoid a divide by zero condition.

STAYSL PNNL has been altered to print output to the XFR file for all energy groups, not just the groups with non-zero flux. This provides a data set that is always the same number of items long (for a given number of groups in the energy grid structure) and facilitates importing the data into a spreadsheet for plot generation.

References

Greenwood, L.R., and C.D. Johnson. 2013. *User Guide for the STAYSL PNNL Suite of Software Tools*. PNNL-22253, Pacific Northwest National Laboratory, Richland, Washington. Available at: http://bioprocess.pnnl.gov/STAYSL_PNNL_Request.htm.

Holden, N.E. 2003. "Neutron Scattering and Absorption Properties." In: *CRC Handbook of Chemistry and Physics, 91st Edition* (Internet Edition 2011), W.M. Haynes, ed., CRC Press/Taylor and Francis, Boca Raton, Florida.

KAPL. 2010. *Nuclides and Isotopes : Chart of the Nuclides, 17th Edition*. Knolls Atomic Power Laboratory, Niskayuna, New York.

Zsolnay, E.M., R.C. Noy, H.J. Nolthenius, and A. Trkov. 2012. *Summary Description of the New International Reactor Dosimetry and Fusion File (IRDFF release 1.0)*. INDC(NDS)-0616, IAEA Nuclear Data Section, Vienna, Austria.

Attachment A - Updated version of Figure 2 from Greenwood and Johnson [2013] for STAYSL PNNL Suite version 1.2.0
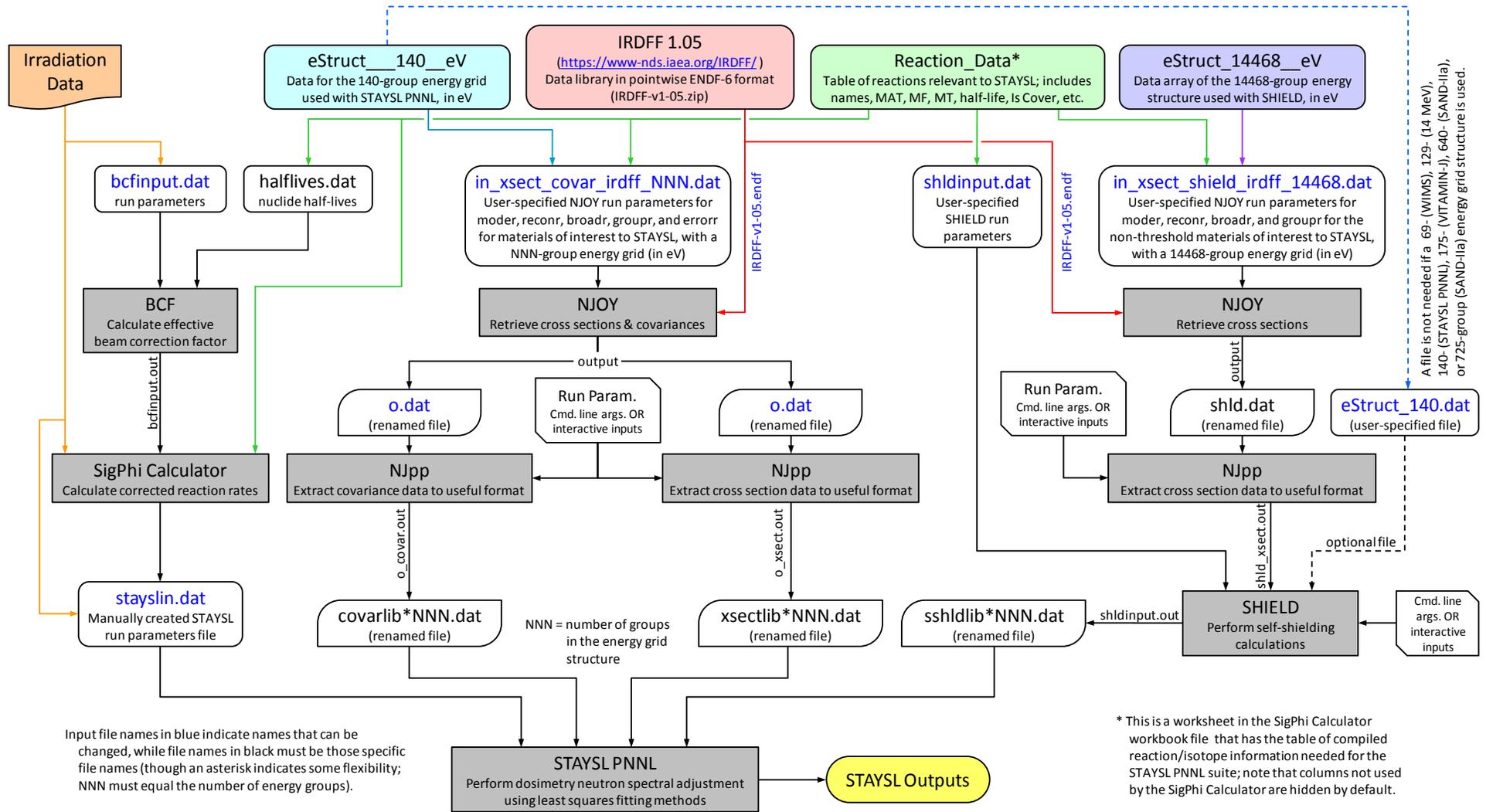

Figure 2. *Detailed relationship between the software tools in the STAYSL PNNL suite, data sources, and input/output files. (Note that NJOY99 is a third-party software that is used in this sequence of data analysis, but whose code is not included in the STAYSL PNNL suite).*