1 Introduction

Fission products are an important observable for basic sciences studying fission products and for a post-detonation nuclear event which may help with attribution and device reconstruction of a nuclear event. The available methods for predicting fission product yields are limited in the energy fidelity and amount of experimental data available to inform evaluations. The purpose of this scripted tool is to alleviate issues with current approaches that utilize a sparse amount of energy dependent data points.

This tool utilizes experimental data and models to predict fission product distributions and yields from short timescale neutron induced fission. A general knowledge of the neutron environment causing fission is required to use this tool, either for a known neutron spectrum or candidate neutron spectrum to test the design space. The predictive ability of this tool reports the cumulative fission product yield of selected isotopes and mass chain yields for uranium or plutonium based environments.

1.1 Usage of Tool

1. Estimation of fission product mass chain yields
2. Estimation of selected fission product cumulative yields where experimental data is available
3. Usable as input for nuclear forensics exercises
4. Verification and validation of known fission products against a candidate neutron spectrum or energy dependent fission spectrum

1.2 Limitations of Tool

1. **Not for nuclear reactors**. Time dependency is not included in this tool.
2. Fissioning energies above 20 MeV

2 Methodology

The key pieces of information relevant to the prediction of fission product yields are the fissioning isotope and neutron energy fluence. A fissioning system, for example ^{235}U (n,f), absorbs a neutron and creates a compound nucleus which can proceed through the fission reaction. In the example case, ^{236}U is the isotope that actually goes through this process. Different fissioning systems have different fission product distributions.

The neutron energy fluence spectrum has a large impact on the fission product distribution. The valley (A 115) and wing (A less than 90 or A greater than 150) fission products are produced with greater yield as the incident neutron energy causing fission is increased. Figure 1 shows an example with ^{235}U (n,f) over the energy data available in ENDF/B-VII.1. The peak isotope yields (A 95 and A 140)are relatively insensitive to incident neutron energy.

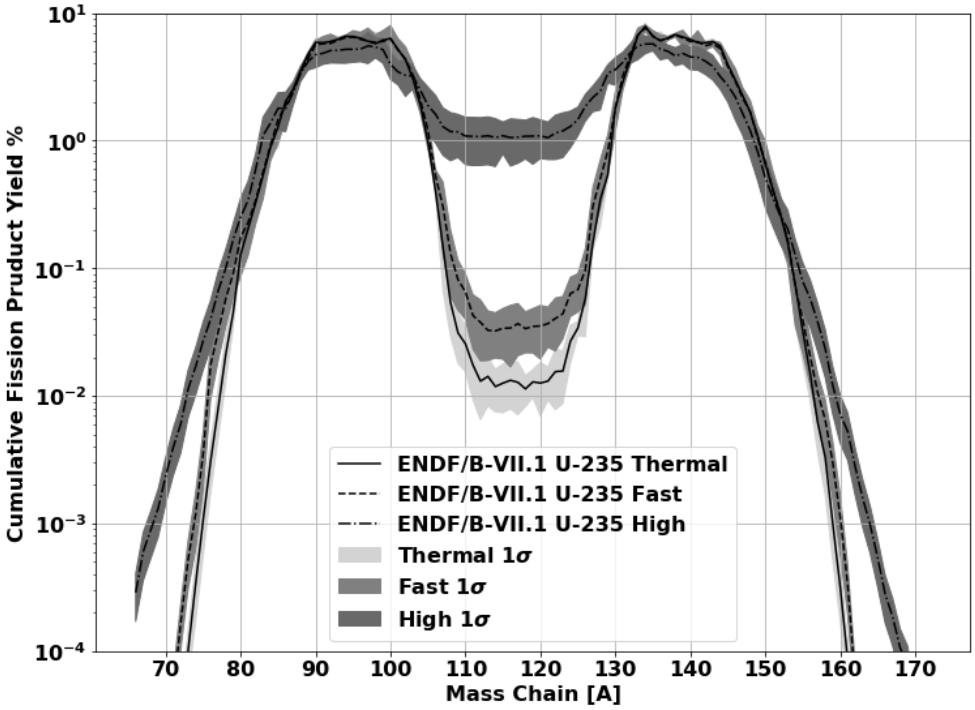

Figure 1: Comparison of energy dependent ^{235}U cumulative fission product distributions from ENDF/B-VII.1 [1].

It is important to note that only these 3 data points at thermal, fast, and high energy are used in most codes that can approximate fission product yields. The problem that this tool addresses is the lack of energy resolution which can lead to incorrect predictions if the neutron energy distribution is not an exact match with

these 3 energy groups.

The actual quantity of interest related to the aforementioned key pieces of information is the fissioning system energy distribution. The neutron energy spectrum convolved with the fission cross-section is proportional to the fission energy distribution. This quantity is generally calculated with Monte Carlo or deterministic based neutron transport codes.

The fissioning neutron energy distribution is utilized in this tool to determine the fission product yield with a phenomenological fit and the General Description of Fission Observables (GEF) code [2]. Including fits to experimental data enables better energy resolution and predictions that are consistent with observed experiments where experimental data exists, while GEF enables predictions for mass chains lacking sufficient energy-dependent data.

2.1 Empirical Fit to Phenomenological Model

Empirical relations developed by Nagy, *et al.* provide an approach to predict the fission product yield as a function of energy given sufficient yield measurement data [3]. Nagy fits the fission product experimental data to the exponential equation

$$Y(E_n) = Y_0 e^{bE_n}, \tag{1}$$

where the fitting parameters b and Y_0 represent the slope of the function in logarithmic form and thermal fission yield, respectively[3]. The slope is the primary measure of the energy dependency of the fission product yield, which required modifications for multi-chance fission. First chance fission is dominant from up to 5.5 MeV, and second-chance fission up to 14.1 MeV[3]. Multi-chance fission effects on the fission product yield are less pronounced in asymmetric regions but can have a large impact in symmetric fission ($109 \leq A \leq 129$) [4, 3].

For this part of the predication tool, the available data is fit to equation 1 within a Monte Carlo simulation sampling of the experimental data. The experimental data are modified over 1,000 trials to determine the error from fitting the data to the fit equation. As should be expected, nuclei that have little experimental values will have worse fits and therefore higher uncertainty.

2.2 GEF

GEF is applicable over a wide range of fissioning systems including isotopes with atomic numbers from 80 to 112[2]. The underlying model has been shown to have good predictive power, albeit with relatively large uncertainties due to up to 50 free parameters, using potential energy surfaces of the fission barrier of the fissioning system, theory, and adjustments based on empirical parameters [5, 6]. GEF incorporates

covariance information of the fissioning system, multi-chance fission, and many other unique features.

The values for the mass chain yield distribution calculated by GEF were determined utilizing separate calculations for each energy group defined by the midpoint bin energy of the fissioning systems for neutron induced fission. The fissioning isotopes calculated were ^{236}U, ^{237}U, ^{238}U, ^{240}Pu, and ^{241}Pu. Note that these are the initial nucleus plus one neutron.

The energy dependent calculations in GEF were completed in the 46 Group DPLUS structure, which is given in the distribution under "*Data\E_Bins.xlsx*".

If the energy spectrum entered into the inputs utilizes this group structure, the result is calculated with matrix multiplications of the stored data from GEF. The actual GEF runs for each isotope take several hours to complete but are precalculated with results included in this tool. The uncertainty reported includes a combination of the GEF Monte Carlo statistical and systematic uncertainty and the uncertainty in the input added in quadrature.

If the energy spectrum used in the input is not the 46 group DPLUS structure, the GEF data is fit to equation 1. This method works for a large proportion of the mass chain yields ; however, there can be large errors fitting the equation for low yield fission products. GEF reports results with five significant figures, so yields below this have rounding truncation error. For this reason, mass chains 56-77 and 155-180 are not reported in the GEF results if the 46 group DPLUS structure is not utilized. These mass chains either could not be fit to the distribution due to the data or uncertainty in the fit was over 150%.

3 Tool

There are 4 main sections that are distributed with the tool. These are the FPPT.exe and the Data, Inputs, Output folders. Additionally, the main Python 2.7 script is included labeled FPPT.py. This includes all of the functions in the script as well as the main driver.

3.1 Data Folder

The Data folder contains both ".pckl" files and '.xlsx" files. The pickle files, '.pckl", are used as data storage. The actual GEF results are 100+ MB, so they have been condensed for this application. There are 5 pickle files. One for each of the fissioning isotopes included in this tool. Inside the pickle files is a dataframe containing a matrix of the yields as a function of incident neutron energy and a matrix of the uncertainties as a function of energy.

The Microsoft Excel files, '.xlsx", contain the energy dependent experimental measurements for the phenomenological empirical fits. The format of the file is that each fissioning isotope is the name of the sheet with the format Z_A_Element. In each sheet there are 4 columns. The first column is the energy of the experimental datapoint. The second column is the absolute yield, so a 6% yield isotope at a given energy has an value of 0.06. The third column is the absolute uncertainty. The fourth column is a reference to the Author and year of publication, but is not required. It is a good idea to know where the data is coming from though!

Data can be added to the Excel files by following this format. The tool only uses the data in the Excel files if the isotope cumulative yield appears in all fissioning isotope datasets. Metastable states do not appear in the preallocated list. To add metestable states, the A identifier must be modified to be distinct from the other datapoints. One way to accomplish this is to add a trailing 1 to the A of the sheet: Z_A1_Element. The available data for ^{235}U and ^{238}U distributed with the tool is summarized in Table 1.

3.2 Inputs FOlder

There are 2 file types that can go into the Inputs Folder. Other files are ignored.

3.2.1 Fissioning system energy distributions: ex: "U235.txt

The input files should be placed in the main directory inside the folder labeled Inputs. 5 files can be read as inputs for the fissioning isotope energy distribution: $U235.txt, U236.txt, U238.txt, Pu239.txt$ and $Pu240.txt$. Each input is analogous to a tally from a Monte Carlo or deterministic radiation transport output.

Table 1: ^{235}U and ^{238}U fission products in FPPT

A	**FP**	**Location**	$\mathbf{t_{1/2}}$	$\mathbf{E_\gamma}$ **[keV]**	$\mathbf{BR_\gamma}$ %
91	^{91}Sr	Light Peak	9.65 hrs	1024.3	33.5
92	^{92}Sr	Light Peak	2.66 hrs	1383.93	90
95	^{95}Zr	Light Peak	64.032 days	756.725	54.38
97	^{97}Zr	Light Peak	16.749 hrs	743.36	93.09
99	^{99}Mo	Light Peak	65.976 hrs	739.5	12.2
103	^{103}Ru	Light Peak	39.247 days	497.085	91
105	^{105}Ru	Valley	4.44 hrs	724.3	47.3
109	^{109}Pd	Valley	13.7012 hrs	88.03	3.67
111	^{111}Ag	Valley	7.45 days	342.13	6.7
112	^{112}Pd	Valley	21.04 hrs	18.5	27
113	^{113}Ag	Valley	5.37 hrs	298.6	10
115	^{115g}Cd	Valley	53.46 hrs	527.901	27.4
132	^{132}Te	Heavy Peak	3.204 days	772.6	77.9
140	^{140}Ba	Heavy Peak	12.7527 days	537.3	24.39
141	^{141}Ce	Heavy Peak	32.511 days	145.4	48.29
143	^{143}Ce	Heavy Peak	33.039 hrs	293.3	42.8
144	^{144}Ce	Heavy Peak	284.91 days	133.5	11.09
147	^{147}Nd	Heavy Wing	10.98 days	531	13.4
149	^{149}Pm	Heavy Wing	35.08 hrs	385.95	3.1
151	^{151}Pm	Heavy Wing	28.4 hrs	340.08	22.5
153	^{153}Sm	Heavy Wing	46.284 hrs	103.2	29.25
156	^{156}Eu	Heavy Wing	15.19 days	1153.8	11.5
161	^{161}Tb	Heavy Wing	6.89 days	25.65	23.2

Each input file contains three columns. The first column is the upper bin boundary for the first energy group starting at the lowest energy. For the DPLUS 46 group structure, this is 4.14E-07 MeV. The energies should be monotonically increasing and the same for every input file. The second column is the number of fissions for the isotope of the input file name in that energy group. The third column is the relative error. Each column is seperated by a comma. The following is an example of the first line of an input: 4.1399E-07,0.00000E+00,0.0000

Only the required inputs for the problem are required. So, if the system only contains ^{235}U, "U235.txt" is the only file needed.

Alternatively, if the neutron flux spectrum is known, it can be converted to the fission spectrum by multiplying by the appropriate fission cross-section. There are a couple methods to accomplish this. There are many energy group formats utilized for nuclear weapon spectra, so it is not very useful to have tabulated cross-sections to multiply by the flux. An appropriate way to accomplish the task of acquiring the fission energy spectrum is through a Monte Carlo radiation transport simulation. Set the source as the neutron spectrum in the direction of a thin layer of the isotope of interest. The ^{235}U fission reaction rate as a function of energy can be calculated in MCNP for a 93.217% enriched ^{235}U with:

FC4 U235 Fission Reaction Rate (Fissions per cm$\hat{3}$ per src particle)
F4:n 6
FM4 (-0.93217 1 -6) $Flux * atom density of material 6 * sigma f
Where the energy bins are set for the entire set of tallies.

3.2.2 "Weights.txt"

This optional file contains the integral number of fissions for each isotope. The primary use for this is to approximate ^{236}U (n,f) as ^{238}U (n,f). Both of these isotopes are threshold fissioners. ^{238}U is much more well studied. If the concentration of ^{236}U is low ($<<$ 1%), this approximation will have negligible impact to the problem.

Below is an example of the file. The example contains ^{235}U and ^{238}U. These values are obtained by the integral number of fissions for each with ^{236}U added to ^{238}U. Normalization is taken care of in the tool, so the magnitude of the values is not important. If this file is used, all of the isotopes must be given a weight, even if it is zero. The following is an example of this input.

U235,2.37690E-03
U236,0.0
U238,2.05990E-05
Pu239,0.0
Pu240,0.0

If this file is absent, the normalization is performed with the fission energy distribution. The weights in that case are a weighted average of the inputs.

3.3 Running the tool

The tool was created with PyInstaller on Windows 10, so it will run on Windows machines. There are 2 methods to execute the tool and an option to use the script directly. To use the tool, run FTTP.exe by double clicking on the executable or run

FTTP.exe on the command line. The last option is to use Python 2 directly. The script used to generate the executable is included in the distribution. The script is setup to be run in the main directory, in the same folder contining Data, Output, and Inputs. Adjustments may be needed if using Python 3 because dictionaries are used in the script. The behavior of the tool is not dependent on how it is executed.

The progress of the tool will be printed to a terminal. The print statements generally only stay if the executable is run from the command line. 2 examples of code progression are shown below in Figures 2 and 3. If the group structure matches the 46 group DPLUS structure, the speed of the tool takes a few seconds, otherwise it is near 30 seconds. The print statements are reflected in the output file as well.

Figure 2: Tool command line response example 1

In the response in Figure 2, the terminal first displays the collection of the GEF results. In this case U-235 and U-238 were in the input. Next, the results are collected and the tool proceeds through the experimental data phase. The [ ] after "Deleted data for" records what experimental data was not available for all fissioning isotopes. In this case, the data appears in both fissioning isotopes from the input.

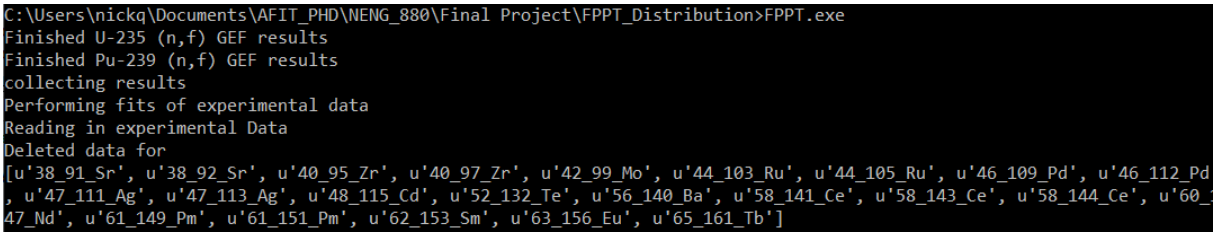

Figure 3: Tool command line response example 2

In the tool response shown in Figure 3, U-235 and Pu-239 are used in the inputs. The print statements are generally the same except for the "Deleted data for" output. Pu-239 did not have data available for the isotopes printed.

3.4 Output

After executing the tool a file formatted as "YYYY_ MM_ DD_ #.txt" will be populated in the Output folder. The output is incremented when used multiple times on

the same day. There are several sections in the output that have been structured for parsing data if needed.

1. First, the weights are reported. The weights sum to unity.
2. Second, the first GEF line will either be "Calculating GEF results with interpolation based on group structure provided" or " Calculating GEF results with DPLUS 46 Group Structure". This print statement reflects if the 46 Group DPLUS structure was used. The next lines provide input on which isotopes were read in from the inputs.
3. Third, the mass chain results from GEF are reported. There are three column following "Mass Chain [A], Mass Chain Yield [%], Mass Chain Yield Uncertainty [%]". The first column is the A of the mass chain. The second column is the yield in percent. The third column is the yield absolute uncertainty in percent.
4. Last, the experiment data results are reported following the text "Experimental Data Results". The reported results have the same format as the GEF results. However, the first column should be interpreted according to the data available in the experimental data in the Data folder.

References

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[2] K. Schmidt *et al.*, "General Description of Observables in Low-energy Fission : GEF Model Code," 2015.

[3] S. Nagy, K. F. Flynn, J. E. Gindler, J. W. Meadows, and L. E. Glendenin, "Mass Distributions in Monoenergetic-Neutron-Induced Fission of U238," *Physical Review C*, vol. 17, no. 1, pp. 163–171, 1978.

[4] J. Bevins, "Targeted Modification of Neutron Energy Spectra for National Security Applications," Ph.D. dissertation, University of California, Berkeley, 2017.

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