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Graphical Post-Processor Created for the ORIGEN2 Code

Prepared for the U.S. Department of Energy
Assistant Secretary for Nuclear Energy

Westinghouse Hanford Company Richland, Washington

Hanford Operations and Engineering Contractor for the
U.S. Department of Energy under Contract DE-AC06-87RL10930

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GRAPHICAL POST-PROCESSOR CREATED FOR THE ORIGEN2 CODE

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ABSTRACT

ORIGEN2[1] is an isotope generation and depletion code developed at the Oak Ridge National Laboratory. It is commonly used to determine the isotopic activity, concentration, and heating as a function of irradiation and decay time. Additionally, ORIGEN2 calculates the gamma-ray and neutron source as a function of time. Because the output generated by ORIGEN2 is often very large, a post-processor was created for ORIGEN2 to graphically display the isotopic concentration (g), activity (C), and decay heat (W) as a function of time. By making the ORIGEN2 output available in a graphical form, the scientists can better understand their calculations and browse through the output to graph important results.

I. INTRODUCTION

The ORIGEN2 graphical post-processor was created using the PV-Wave[a] software operating on a SUN[b] workstation. The software remains in the development stage and is modified routinely to improve its capabilities. This paper contains an overview of the latest developments and plans for future upgrades.

PV-Wave is a software package designed to plot and visualize large data sets in two and three dimensions. It also has a programming language with the capability of displaying menus for user interaction. In order to use PV-Wave, it must be running on the system.

The current program was developed on a SUN Sparc[c] workstation. PV-Wave will operate in both the Sunview[d] and X-Window[e] (open windows 2) environments. The program will process small ORIGEN2 output files with only 8 megabytes of memory. However, larger ORIGEN2 outputs have run up against the memory limit on a workstation with 16 megabytes of memory. Additionally, because of the large amount of input processing that must be performed, the program requires significant time (15 min for a 10,000-line file) to read in large output files. Future upgrades will address this issue.

The post-processor directly reads from the ORIGEN2 output file and does not require any changes to the ORIGEN2 source code. It would be more efficient to have ORIGEN2 interface directly with PV-Wave, or have ORIGEN2 create data arrays to be read by PV-Wave and thus remove the input parsing routine from the PV-Wave command structure. To improve the efficiency, the code will eventually be upgraded to have PV-Wave execute a C program which will format the ORIGEN2 output data into arrays which can be read by PV-Wave.

The current version of PV-Wave parses the ORIGEN2 output file and stores the curie inventories, composition, decay heat, photon source, and neutron source. Because of the processing limits, the program does not access the other ORIGEN2 output tables. Later versions of the code will include the capability of processing multiple tables.

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[a]PV-Wave is a trademark of Precision Visuals, Inc.

[b]SUN is a trademark of Sun Microsystems, Inc.

[c]SUN Sparc is a trademark of Sun Microsystems, Inc.

[d]Sunview is a trademark of Sun Microsystems, Inc.

[e]X-Window is a trademark of the Massachusetts Institute of Technology.

II. DESCRIPTION OF THE ORIGEN2 GRAPHICAL POST-PROCESSOR

After the data is read in, the user can manipulate it with the menu interface. Figure 1 is a list of the PV-Wave menus available in PV-Wave for plotting ORIGEN2 output data.

Figure 2 is a layout of the windows and menus. The window in the lower left portion of this figure contains the PV-Wave program commands and execution status. All PV-Wave warning messages are displayed and user input is entered in this window. Note that the commands required to run the program and the responses to questions asked by the program (including the name of the ORIGEN2 output file to process) are in this window.

The plot window takes up the majority of the screen. All plots are displayed in this window. It can be resized and moved like any other workstation window. Below the plot window is the message window used by the program to inform the user of various errors. To the left of the plot window are the main menu options as outlined in Figure 1.

The basic capabilities are linear plots and log plots of the mass, curie inventory, or decay heat. Multiple isotopes can be plotted on the same graph using the "OVERPLOT" command. The user can display up to nine plots on the screen to provide easy comparisons.

The user has control of the x range and y range and can change the time units on the x axis. A modest number of symbols can be attached to the lines. On a color terminal, the plot lines are colored to help differentiate between the lines.

There are currently two methods to plot the mass, curie inventories and decay heat. The program will plot the major contributors or individual isotopes can be selected for plotting. When the program plots the major contributors, the user must select a percentage of the major contributors. For example, by selecting 10%, the program will display the top 10% of the isotopes that contribute to the mass, curie inventory, or decay heat. By selecting 100%, all of the isotopes are plotted. The program plots the major contributors over all time intervals, starting from the highest and working toward the lowest. The order in which the line plots are displayed indicates their relative importance.

Figure 3 is a plot generated by requesting the program to plot the top 80% of the isotopes that contribute to actinide curie inventories. The commands to generate this plot are shown in the upper right corner. The total inventory is the black solid line at the top of the plot. Note that ^{239}Np is the major contributor during irradiation, but it decays quickly after shutdown leaving ^{241}Pu as the major curie source.

The user may select individual isotopes to plot from a list of the available isotopes. Additional isotopes are plotted on the same graph using the "OVERPLOT" command in the main menu.

Figure 4 is a plot of selected isotopes. These isotopes are of importance for relatively long decay times after the reactor has shut down. Figure 5 is a similar plot of the primary contributors to the decay heat in the first days following shutdown (of the reactor).

A particularly useful feature of the code is plotting the neutron and photon source as a function of time. The user can select the (α,n) neutron source, the spontaneous fission source, or both. The code will also plot the isotopes that contribute to the neutron source, allowing the user to quickly identify the major contributors and see their time dependent behavior.

Figure 6 is a plot of the contributors to an (α,n) neutron source. Note that ^{239}Pu is the main contributor. Figure 7 is a plot of all of the contributors to the spontaneous fission neutron source. The primary contributor is ^{240}Pu. In fact the ^{240}Pu spontaneous fission source is higher than the total (α,n) source shown in Figure 6.

There are two methods of plotting a photon source. The first is a plot of the source as a function of energy for a specific decay time. This provides an easy method of plotting the photon spectra. The user can overplot the gamma ray energy spectra at various decay times for comparison. Additionally the program will graph, on the same plot, the total photon spectra for the actinides, activation products, and fission products.

Figure 8 shows a plot of the energy dependent photon source for five decay times. This is a log - log plot of source intensity at specific decay times as a function of gamma ray energy in megavolts. Reactor shutdown is at 100 days.

The second method is a three-dimensional plot of the photon source as a function of energy and time. When this plot is displayed, the user may rotate the plot in segments of 10 degrees, either left, right, up, or down. There may be other ORIGEN2 data that could be

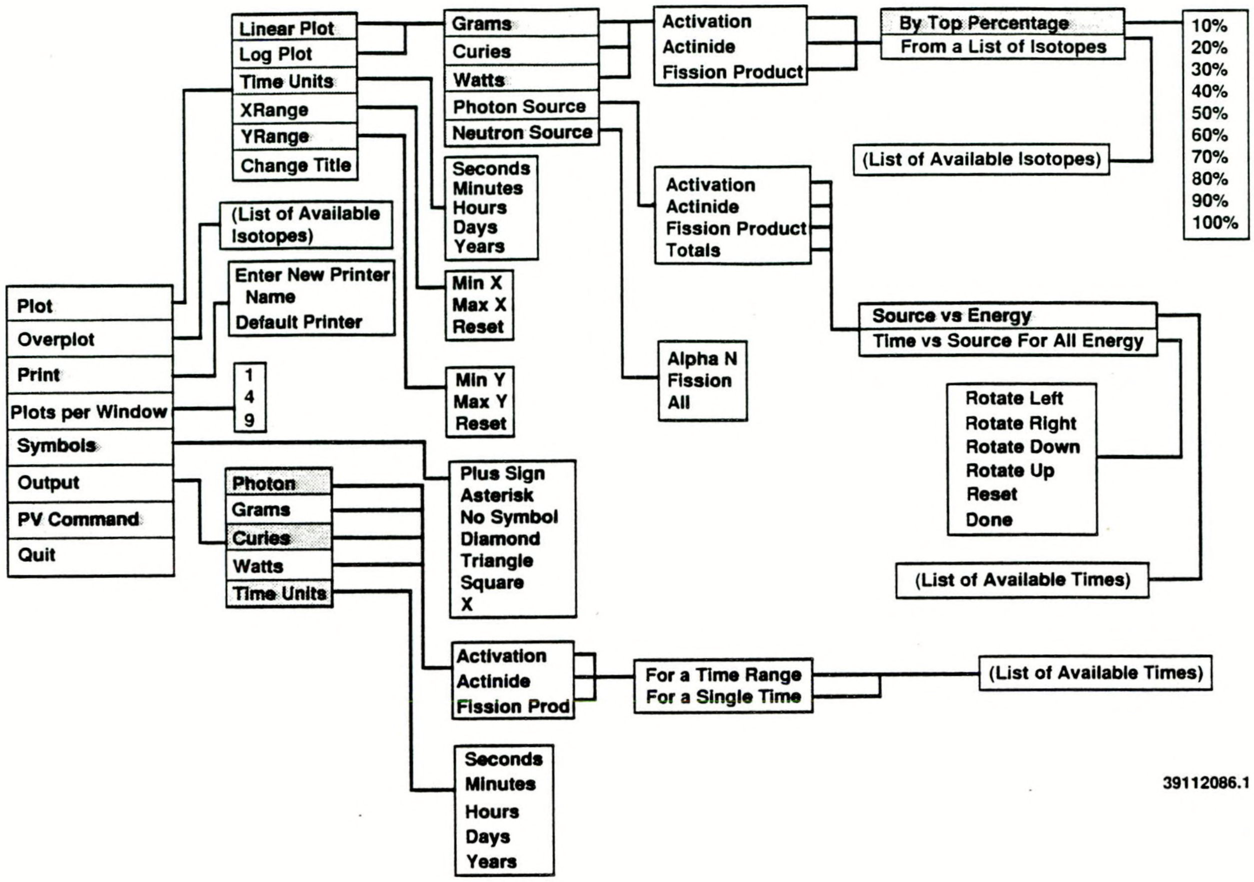

Fig. 1. Menus Available in the ORIGEN2 Post-Processor

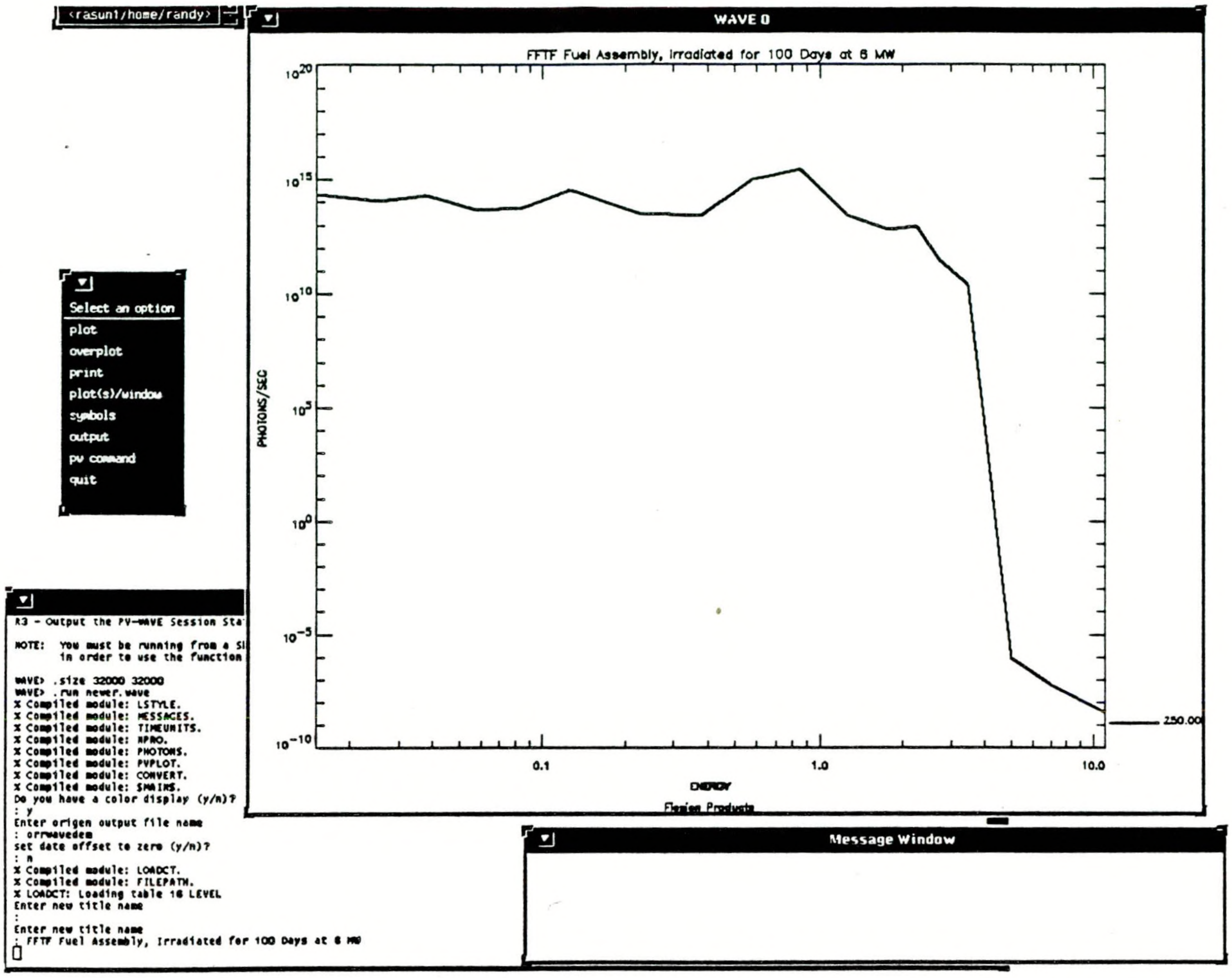

Fig. 2. Screen Layout for the ORIGEN2 Post-Processor

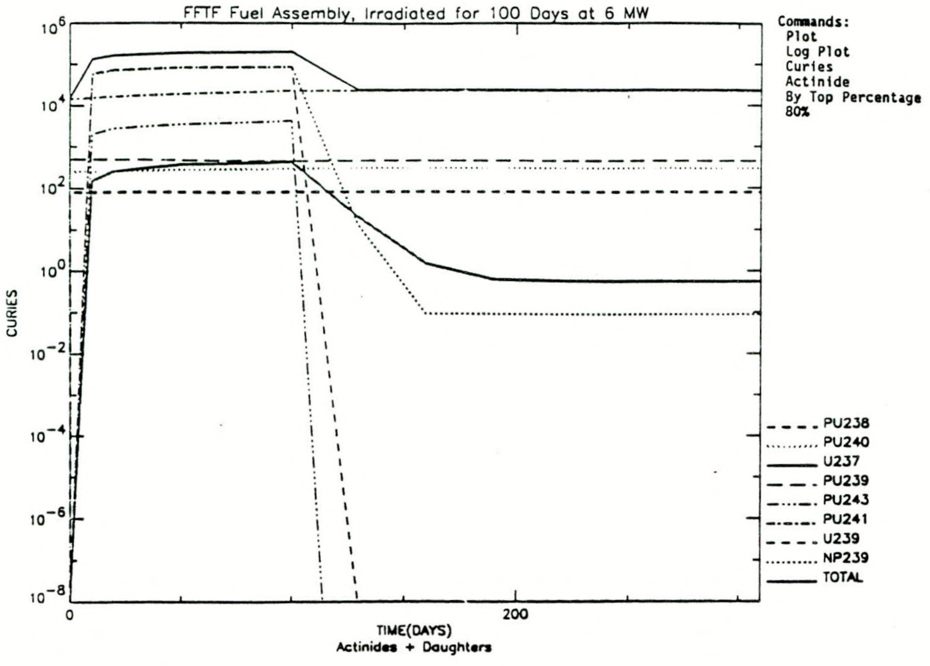

Fig. 3. Plot of the Major (Top 80%) Isotopes that Contribute to the Actinide Curie Inventory

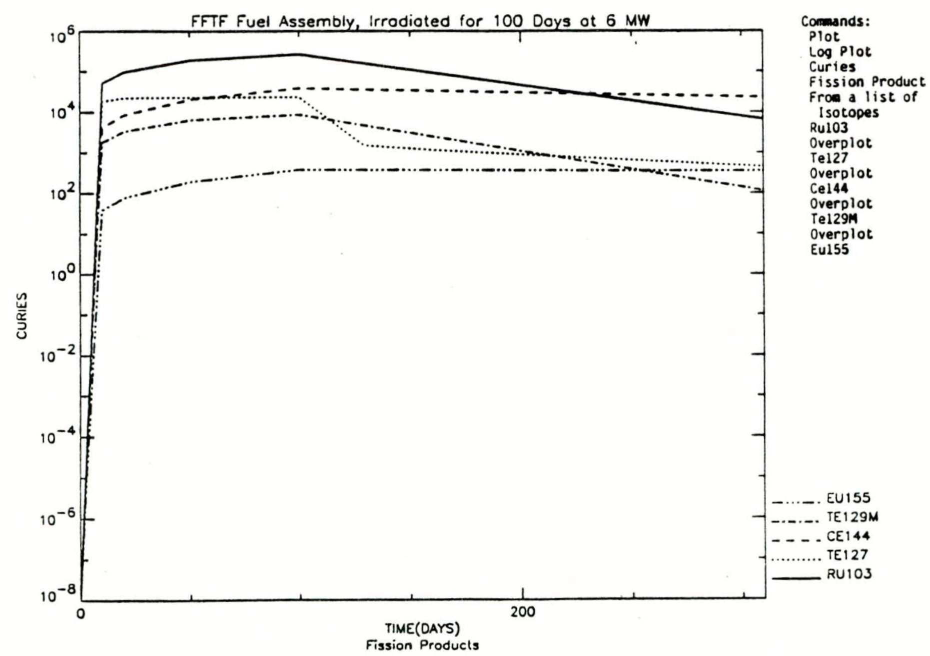

Fig. 4. Plot of Selected Isotopes that Contribute to the Fission Product Curie Source

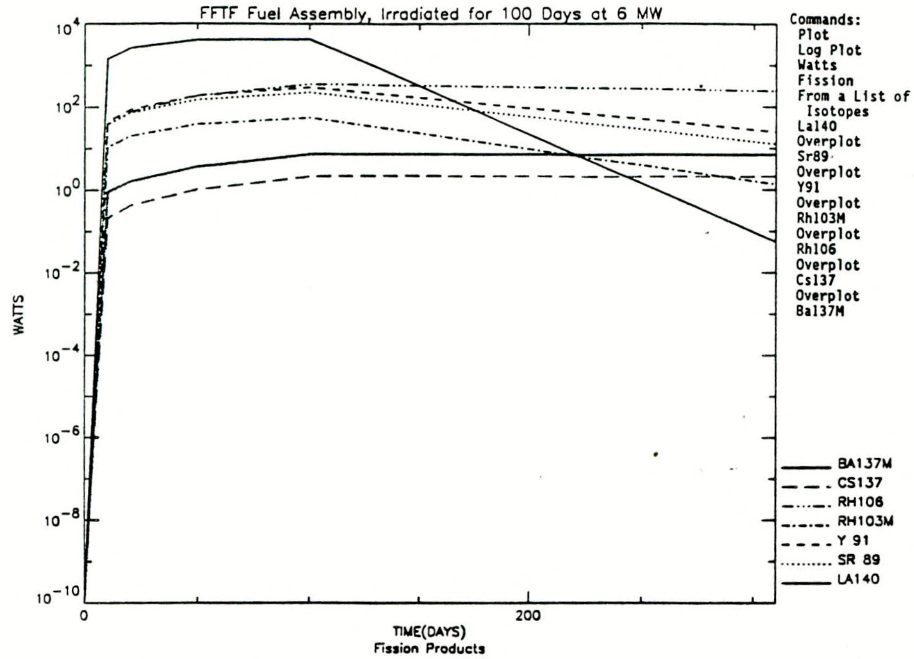

Fig. 5. Plot of Selected Isotopes that Contribute to the Fission Product Decay Heat

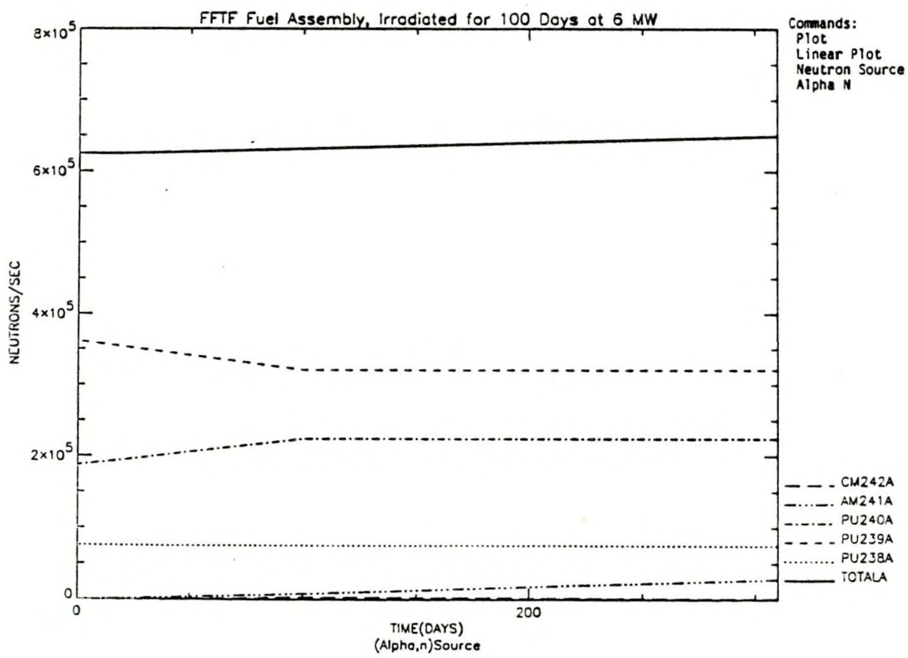

Fig. 6. Plot of the (Alpha,n) Neutron Source

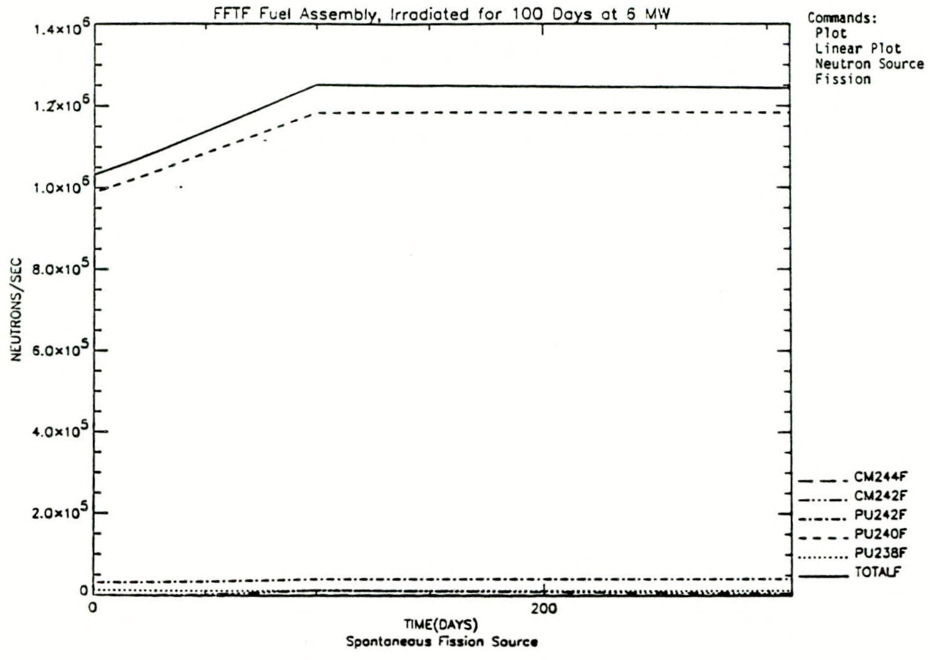

Fig. 7. Plot of the Spontaneous Fission Neutron Source

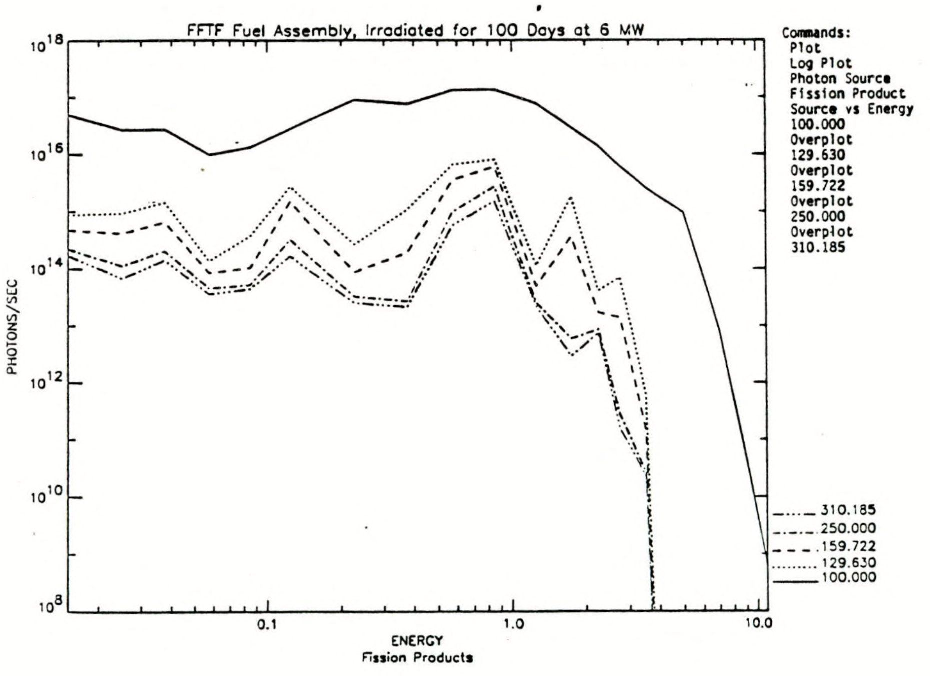

Fig. 8. Plot of the Energy Dependent Photon Source

better visualized using three-dimensional plots, however, the photon source is currently the only data that can be processed in three dimensions.

The program also allows the user to write out the neutron and photon source, mass inventories, curie inventories, and decay heat information to an ASCII file for input to documents or other computer codes. These tables may be written for specific times or over a range of times.

III. FUTURE UPGRADE OPTIONS

This graphical processor is still in the development stage and a number of features are planned. For example, it is possible to animate the values from ORIGEN2 as a function of time. This would allow the user to monitor the buildup and decay of isotopes in a short animated sequence.

Future upgrades will also visualize the gram inventories, curie inventories, and decay heat values in three dimensions. For these cases the independent variables would be the various isotope selections and decay time.

Other planned upgrades include displaying the isotopic photon source for each energy group and adding curve fitting options.

IV. CONCLUSION

The use of visualization techniques to better understand and display scientific data is vital to the continual evolution of the scientific computing environment. By using these methods, the scientist and engineer are provided with a tool that allows them to quickly assimilate calculated results and better understand the data that has been generated.

V. REFERENCES

1. A. G. CROFF, *A User's Manual for the ORIGEN2 Computer Code*, ORNL/TN-7175, Oak Ridge National Laboratory, Oak Ridge, Tennessee, (1980).

DISTRIBUTION

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