Easy-to-use Application Programs to Calculate Aggregate Fission-Product Properties on Personal Computers

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Fission Products (FP) are dominant sources of activities in spent nuclear fuels over tens of years. Small Fortran programs for personal computers have been developed primarily to study the aggregate FP decay heat and delayed-neutron activities with the latest fission yield and decay data in Japanese, US and European Nuclear Data libraries. This paper describes how to use these programs together with two new features of our codes; i) unified front-end ii) capability of calculating the aggregate β and γ decay energy spectra.

1. Introduction

Fission products (FP) are inevitable by-products which are primary sources of activities in spent nuclear fuels for about 30 years (=10^9 s). Hence, the fission-product properties are not only key nuclear data required in designing the nuclear fuel cycle, but also of interest of the general public who are not working in the nuclear industry

In our fission-product studies, we have developed and utilized programs on personal computers for calculating the aggregate decay heat and the aggreagete delayed neutron emission as functions of cooling times. The calculations in the codes are based on the summation method and use fission yields and decay data in three major nuclear data libraries, JNDC nuclear data library of fission products version 2 (Japan), ENDF/B-VI (USA) and JEF2.2 (Europe).

These computer codes can calculate decays of about 1000 fission product nuclides after a fission burst or finite irradiation for a single fissile nuclide. One may calculate the following FP properties as functions of cooling time; concentrations of radioactive FP's, aggreagate FP decay heat, aggregate delayed neutron emission, and aggregate (β and γ) decay energy spectra. The calculations can be performed for 51 fissioning systems when one uses ENDF/B-VI fission yield data.

In the present release of the codes, previously developed small separate programs are unified in a compact form in order to improve operational easiness, and the β and γ decay energy spectra can now be calculated.

2. Features

Capable to calculate the aggregate β and γ decay energy spectra

In the present release, the aggregate β and γ decay energy spectra can be calculated, too.

The FP properties that can be calculated with the code is summerized in Table 1.

New unified front-end

A unified user-friendly control panel is provided for the six programs.

Easy data transfer

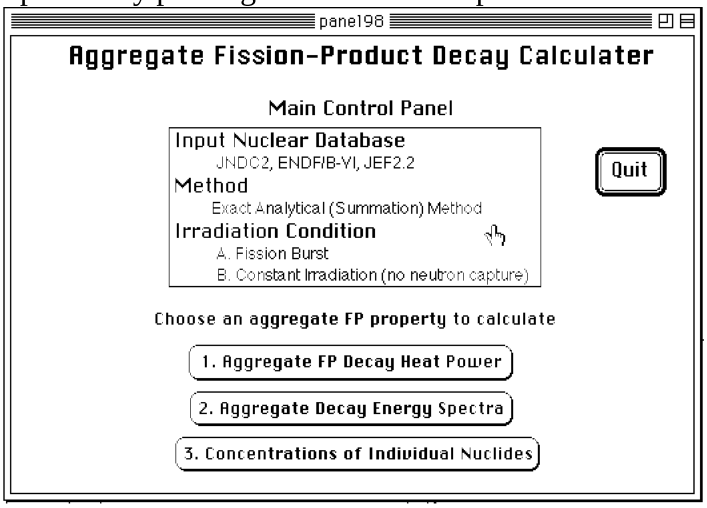
The output files are text files. Therefore, the output data can be easily transferred to Excel (Microsoft Corporation), Transform (Fortner Research LLC) or any other application programs for detailed analyses.

3. Quick start

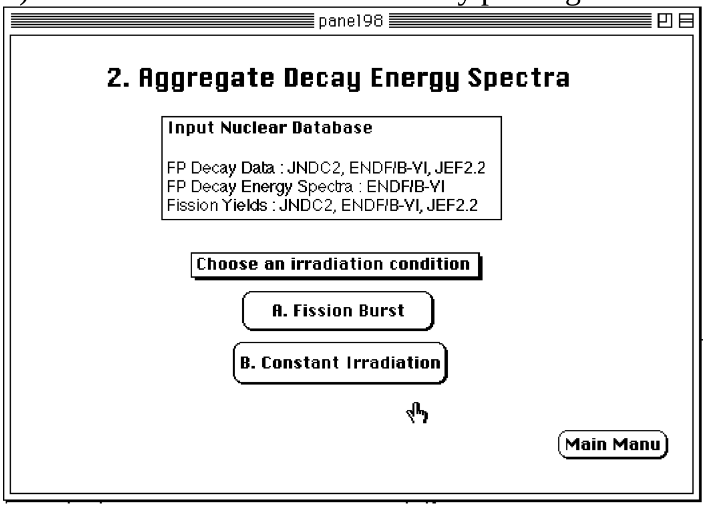
In the following, we describe how to calculate the aggregate decay energy spectrum after a finite irradiation. One can perform other calculations easily in the same way.

Note : A cooling time file should be prepared beforehand when one calculate the aggregate decay heat powers ("1. Aggregate Decay Heat Power" in the Main Control Panel). See also Sect. 6 b).

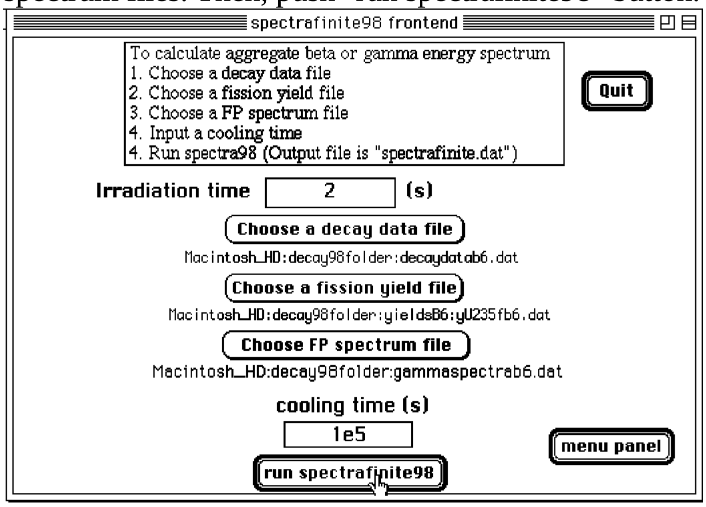
1) Open a HyperCard stack named "panel98", and choose "2. Aggregate Decay Energy Spectra" by pushing the button in the panel.



2) Choose an irradiation condition by pushing a button in the panel.



3. Enter irradiation time and cooling time in the boxes, and choose fission-yield, decay-data, and spectrum files. Then, push "run spectrafinite98" button.



4. Input FP nuclear data

The FP nuclear data required in the codes are categorized into three;

a) fission yield data

y_i independent fission yield of FP nuclide i

b) decay data

$b_{i \to j}$ branching ratio of FP nuclide i decaying to nuclide j

λ_i decay constant of FP nuclide i

E_i average decay energy per decay of nuclide i

$P_{n\,i}$ delayed neutron emission probability of nuclide i

c) spectrum data

$\chi(E)$ decay energy spectrum of nuclide i (ENDF/B-VI only)

The present codes can perform calculations with the above data in ENDF/B-VI, JNDC 2 and JEF2.2. It is noted that the input FP data for a calculation can be taken from different libraries. For example, one may use the fission yields in JEF2.2 and the decay data in JNDC2 to calculate the aggregate decay heat powers.

5. Numerical method

The codes solve analytically decays and buildups of FP nuclides. The definitions of the irradiation conditions, a fission burst and constant (finite) irradiation, are shown in Fig. 1. Specifically, the equations for the concentration of nuclide i, $N_i(t)$, is given as follows;

a) fission burst

$$\frac{d}{dt}N_i(t) = -\lambda_i N_i(t) + \sum_{j \neq i} b_{j \to i} \lambda_j N_j(t) ,$$
$$N_i(0) = y_i \ .$$

b) constant (finite) irradiations

For simplicity, the codes utilize the solution for infinite irradiation. Therefore, concentrations of the stable nuclides can not be calculated with the present codes. The concentration of nuclide i, $N_{\infty i}(t)$, after infinite irradiation is obtained from

$$\frac{d}{dt}N_{\infty i}(t) = -\lambda_i N_{\infty i}(t) + \sum_{j \neq i} b_{j \to i} \lambda_j N_{\infty j}(t) \ ,$$
$$N_{\infty i}(0) = Y_i / \lambda_i \ .$$

Here, Y_i is the cumulative fission yield of nuclide i, defined as

$$Y_i = y_i + \sum_{j \neq i} b_{j \to i} Y_j \ .$$

Finally, the concentration of radioactive nuclide i, $N_i(t)$, after irradiation time T (see Fig. 1) is given by

$$\boldsymbol{N}(t) = \boldsymbol{N}_\infty(t) - \boldsymbol{N}_\infty(t+T) \ .$$

6. Program and data files

a) program files

panel98 Main control panel (HyperCard stack). The following six programs are called from this panel.

decay98, decayfinite98, distel98, distelfinite98, spectra98, spectrafinite98

These six calculation programs are called from "panel98". Therefore, users do not have to open directly these programs.

b) cooling time file for aggregate decay heat calculations

To use "decay98" and "decayfinite98", one should prepare a text file which contains the arbitrary number of cooling times with an arbitrary file name. The file named "egct.dat" is a sample cooling time file.

c) fission yield files and folders

Fission yield files are stored in the following three folders;

yieldsB6	ENDFB/VI fission yield folder
yieldsJNDC2	JNDC fission yield folder
yieldsJEF2.2	JEF2.2 fission yield folder

The nomenclature of the files is as follows;

(file name)="y"+(isotope)+(isomeric state)+(neutron energy)+(library name)+".dat".

(isomeric state) = "M" used only for a fissile in an excited state.

(neutron energy) = "t" (thermal), "f" (fast), "h" (14 MeV), s (spontaneous).

(library name) = "b6" (ENDF/B-VI), "jndc2" (JNDC2), jef22 (JEF2.2).

d) decay data files ($b_{i \to j}$, λ_i , E_i , $P_{\mathrm{n}\,i}$)

decaydatab6.dat	decay data from ENDF/B-VI
decaydatajndc2.dat	decay data from JNDC2
decaydatajef22.dat	decay data from JEF2.2

e) spectrum files

betaspectrab6.dat	FP β spectra from ENDF/B-VI
gammaspectrab6.dat	FP γ spectra from ENDF/B-VI

f) miscellaneous files

egct.dat	sample cooling time file for decay98 and decayfinite98
nameofelements.dat	element names
rtyp.dat	reaction types
InputFiles	work file created by "panel98"

7. Output files

a) decayheat.dat (decay98) and decayfinite.dat (decayfinite98)

time (s), t*Pb (MeV), t*Pg (MeV), t*Pa (MeV), t*d.n.act.

The symbols Pb, Pg and Pa stand for the aggreagte β, γ and α decay heat powers, respectively, while "d.n.act." indicates the aggreagte delayed neutron activity. These powers and activity are multiplied by cooling time "t" in the output file.

b) distel.dat (distel98) and distelfinite.dat (distelfinite98)

N Z A M isotope yield Pb (MeV/s) Pg (MeV/s) Pa (MeV/s) d.n.(1/s)

For each isotope identified by N, Z, A and M (ismeric state), its β, γ and α decay heat powers are tabulated together with its delayed neutron activity.

c) spectra.dat (spectra98) and spectrafinite.dat (spectrafinite98)

Energy range (MeV) Eav (MeV) Spectra

"Energy range" defines the energy bin with "Eav" being its median. "Spectra" indicates the aggregate β or γ spectrum. The aggregate spectrum is normalized to the aggregate decay heat power.

8. Remarks

The present programs described in this paper is available upon request to the author. They can be used and freely distributed if no part of the programs or data is modified.

The author keeps the copyright of the above programs described in this paper. However, he is not responsible to any damages due to the use of these programs.

Lastly, we welcome any suggestions and helps for the future development of the programs. The codes have been used for the researches on the aggregate FP properties. We are now planing to run the codes on other PC systems than Macintosh and utilize them for educational purposes.

Table 1. List of the codes and their outputs.

code	irradiation	cooling time	output
decay98	fission burst	multiple	aggregate decay heat power and delayed-neutron activity
decayfinite98	constant (finite)	multiple	
distel98	fission burst	single	individual FP yields, decay-energy releases and delayed-neutron emission
distelfinite98	constant (finite)	single	
spectra98	fission burst	single	aggregate β or γ decay-energy spectra
spectrafinite98	constant (finite)	single	

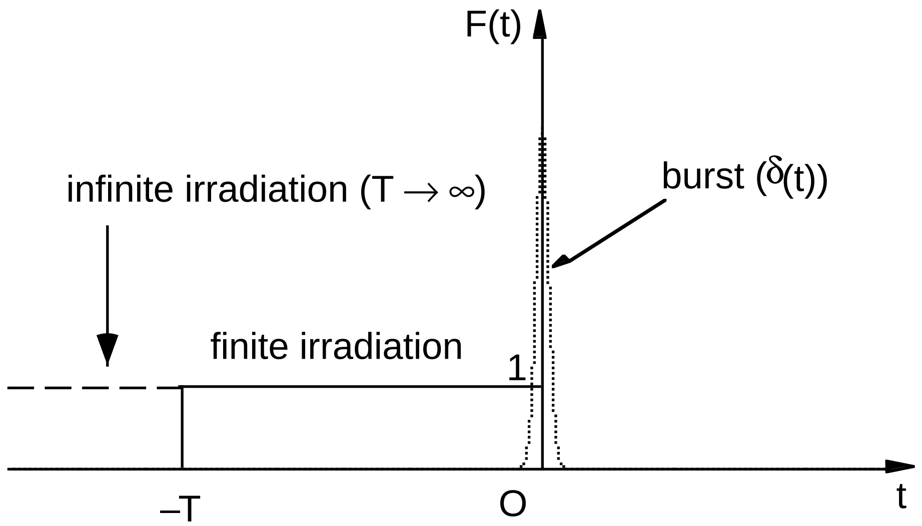


Fig. 1. Definitions of irradiation time and cooling time. The fission rates for the three irradiation conditions are shown as functions of time. Infinite irradiation is defined as the limitting case of the finite irradiation with $T \to \infty$.