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SUBJECT: A Simple Formula for Computing Fission Product
Thermal Cross Sections and Resonance Integrals
TO: Distribution
FROM: C. W. Nestor

SUMMARY

Recently, the results of a number of detailed calculations of fission product thermal cross sections and resonance integrals were published.¹ This memorandum gives a simple formula (and the necessary constants) for computing fission product thermal cross sections and resonance integrals as a function of exposure; the results of this formula agree with those of the detailed calculations to within four percent. The simple formula was used in calculating the effective cross section and resonance integral as functions of fuel-processing cycle time in fluid-fueled reactors.

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192 001

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A SIMPLE FORMULA FOR COMPUTING FISSION PRODUCT THERMAL CROSS SECTIONS AND RESONANCE INTEGRALS

C. W. Nestor

Method

As discussed in reference 1, the contribution C_i of an individual fission product with effective cross section $\hat{\sigma}_i$ and yield y_i to the aggregate fission product cross section σ_{fpa} is given by

$$C_i = y_i \hat{\sigma}_i \frac{1 - e^{-\alpha_i F}}{\alpha_i F} \quad (1)$$

where

$$F = \int_0^t \hat{\sigma}_f \phi \, dt ; \text{ fissions per fissile atom}$$

$$\alpha_i = (1 - P) \frac{g \sigma_o}{g_f \sigma_f} + P \frac{\Sigma_\mu}{\Sigma_f} ,$$

$$P = \frac{\text{nonthermal fissions}}{\text{total fissions}}$$

$$\hat{\sigma} = \text{microscopic effective cross section, barns}$$

$$\sigma_o = 2200 \text{ meter/sec microscopic cross section, barns}$$

$$g = \text{Westcott correction factor for Maxwell-Boltzmann averaged cross section}$$

$$f = \text{subscript indicating fission, e.g., } \hat{\sigma}_f \text{ is the microscopic effective fission cross section}$$

$$\mu kT = \text{energy at which the } 1/E \text{ tail is cut off}$$

$$\Sigma_\mu = \int_{\mu kT}^{\infty} \sigma(E) \frac{dE}{E}$$

$$\Sigma_f = \int_{\mu kT}^{\infty} \sigma_f(E) \frac{dE}{E}$$

If we attempt to lump all the fission products into one pseudo element, we may write

$$\frac{Z}{Z_0} = \frac{1 - e^{-\alpha F}}{\alpha F} \quad (2)$$

where Z is either the fission product aggregate thermal cross section, $g \sigma_0$, or the fission product aggregate resonance integral, RI , and Z_0 is its value at $F = 0$.

The approximation used in this memorandum is

$$\frac{Z}{Z_0} = \frac{1}{1 + F(a_0 + a_1 P)} ; \quad (3)$$

this follows from the useful approximation

$$e^{-x} \approx \frac{1 - \frac{x}{2}}{1 + \frac{x}{2}}$$

and the definition of α . A least-squares fit for a_0 and a_1 can be obtained by writing

$$y = \frac{1}{F} \left(\frac{Z_0}{Z} - 1 \right) ;$$

we obtain

$$y = a_0 + a_1 P .$$

If N is the number of points, then

$$\begin{aligned} a_0 N + a_1 \sum_{i=1}^N P_i &= \sum_{i=1}^N y_i \\ a_0 \sum_{i=1}^N P_i + a_1 \sum_{i=1}^N P_i^2 &= \sum_{i=1}^N P_i y_i \end{aligned} \quad (4)$$

For the points listed in Tables 8 through 10 of Ref. 1, omitting those with $F = 0$, we have $N = 20$, $\sum_1 P_1 = 4$ and $\sum_1 P_1^2 = 1.2$; equations (4) then have the solutions

$$\begin{aligned} a_1 &= 2.5 \left[\sum_1^N y_1 P_1 - 0.2 \sum_1^N y_1 \right] \\ a_0 &= 0.05 \left[\sum_1^N y_1 - 4a_1 \right] \end{aligned} \quad (5)$$

Results

Computed values for the cross sections and resonance integrals are presented in tables 1 through 6 along with the constants used in the computation and the values of the cross sections and resonance integrals from Ref. 1; the percentage deviation of the results of this calculation from those of Ref. 1 is also given. In general, the agreement between the two calculations was excellent.

Application

In a fluid fuel reactor with constant flux and fuel loading, and continuous processing with cycle time θ , the macroscopic poison cross section Σ is given by²

$$\Sigma = y N_f \hat{\sigma}_f \phi \int_{-\infty}^t \sigma_p(t-\tau) e^{-\frac{(t-\tau)}{\theta}} d\tau \quad (6)$$

where N_f is the concentration of fissile material (atoms/b-cm), $y N_f \hat{\sigma}_f \phi d\tau$ is the number of fission product atoms produced in a time interval $d\tau$, $\sigma_p(t-\tau)$ is the effective microscopic absorption cross section at time t of fission-product atoms formed at time τ , and $e^{-\frac{(t-\tau)}{\theta}}$ is the probability that atoms formed at time τ will be in the reactor at time t .

The effective cross section $\sigma_p(t)$ is given by

$$\sigma_p(t) = \frac{1}{y N_f \hat{\sigma}_f \phi} \frac{d \Sigma_b}{dt} \quad (7)$$

where Σ_b is the macroscopic fission product absorption cross section for "fixed" fission products obtained from

$$\Sigma_b = y N_f \sigma \frac{1-e^{-\alpha F}}{\alpha} \quad (8)$$

The "fission product aggregate" microscopic cross section σ_{fpa} is defined as

$$\sigma_{fpa} = \frac{\Sigma_b}{F N_f} = y \sigma \frac{1-e^{-\alpha F}}{\alpha F} \quad (9)$$

i.e., the macroscopic absorption cross section for fission products divided by the total number of fissions. From (9) we have

$$\Sigma_b = F N_f \sigma_{fpa} ;$$

combining this with

$$\frac{d \Sigma_b}{dt} = \frac{d \Sigma_b}{dF} \frac{dF}{dt}$$

and

$$\frac{dF}{dt} = \hat{\sigma}_f \phi ,$$

we have

$$\sigma_p(t) = \frac{1}{y} \left[\sigma_{fpa} + F \frac{d\sigma_{fpa}}{dF} \right] \quad (10)$$

Formula (3) can be written

$$\sigma_{fpa} = \frac{\sigma(0)}{1 + bF}$$

with

$$b = a_0 + a_1 P.$$

For constant P we have

$$\Sigma = N_f \int_0^\infty \left[\sigma_{fpa} + F \frac{d\sigma_{fpa}}{dF} \right] e^{-\frac{F}{\hat{\sigma}_f \phi \theta}} dF$$

$$\Sigma = \frac{N_f \sigma(0)}{a_0 + a_1 P} e^x E_2(x) \quad (11)$$

where $x = \frac{1}{\hat{\sigma}_f \phi \theta (a_0 + a_1 P)}$

$$E_2(x) = x \int_x^\infty e^{-t} \frac{dt}{t^2}.$$

From the definition of $E_2(x)$ we can show that

$$e^x E_2(x) \leq \frac{1}{x}$$

so that

$$\Sigma \leq N_f \hat{\sigma}_f \phi \theta \sigma(0) \quad (12)$$

The right-hand side of Eq. 12 is the cross section due to the fission products generated during one cycle time, assuming no variation of microscopic cross section with time. The quantity $\hat{\sigma}_f \phi \theta$ is the number of fissions per atom of fuel material in one cycle time.

To illustrate the use of Eq. 11, values of $\frac{\Sigma}{N_f \sigma(0)}$ are plotted versus $\hat{\sigma}_f \phi \theta$ in Fig. 1 for U^{235} fission products with $P = 0.2$.

Table 1. Thermal Cross Section ($g \sigma_0$) for U^{233} Fission Products

$$Z_0 = 37.04 \text{ barns}$$

$$a_0 = 0.1883$$

$$a_1 = 0.1050$$

P	F	$g \sigma_0$ (formula 3) (barns)	$g \sigma_0$ (ORNL-2869) (barns)	(δ , %)
0	0.5	33.85	33.90	-0.1
0	1.0	31.17	31.23	-0.2
0	1.5	28.88	28.93	-0.2
0	2.0	26.91	26.94	-0.1
0.1	0.5	33.69	33.72	-0.1
0.1	1.0	30.90	30.89	-
0.1	1.5	28.53	28.47	0.2
0.1	2.0	26.50	26.37	0.5
0.2	0.5	33.53	33.55	-0.1
0.2	1.0	30.63	30.59	0.1
0.2	1.5	28.19	28.08	0.4
0.2	2.0	26.11	25.94	0.7
0.3	0.5	33.37	33.41	-0.1
0.3	1.0	30.37	30.37	0
0.3	1.5	27.86	27.79	0.4
0.3	2.0	25.73	25.63	0.4
0.4	0.5	33.21	33.26	-0.2
0.4	1.0	30.11	30.13	-0.1
0.4	1.5	27.53	27.58	-0.2
0.4	2.0	25.36	25.40	-0.2

Table 2. Resonance Integral (RI) for U^{233} Fission Products

$$Z_0 = 134.34 \text{ barns}$$

$$a_0 = 0.1297$$

$$a_1 = 0.6351$$

P	F	RI (formula 3) (barns)	RI (ORNL-2869) (barns)	(δ , %)
0	0.5	126.16	126.91	-0.6
0	1.0	118.92	118.94	0
0	1.5	112.46	112.46	0
0	2.0	106.67	106.66	0
0.1	0.5	122.51	122.38	0.1
0.1	1.0	112.59	112.37	0.2
0.1	1.5	104.16	103.74	0.4
0.1	2.0	96.90	96.72	0.2
0.2	0.5	119.05	118.82	0.2
0.2	1.0	106.90	106.61	0.3
0.2	1.5	96.99	96.80	0.2
0.2	2.0	88.77	88.82	-0.1
0.3	0.5	115.80	115.51	0.3
0.3	1.0	101.75	101.50	0.2
0.3	1.5	90.75	90.79	0
0.3	2.0	81.89	82.36	-0.6
0.4	0.5	112.71	112.55	0.1
0.4	1.0	97.09	96.96	0.1
0.4	1.5	85.26	85.64	-0.4
0.4	2.0	76.01	76.94	-1.2

Table 3. Thermal Cross Section ($g \sigma_0$) for U^{235} Fission Products

$$Z_0 = 43.00 \text{ barns}$$

$$a_0 = 0.2050$$

$$a_1 = 0.6526$$

P	F	$g \sigma_0$ (formula 3) (barns)	$g \sigma_0$ (ORNL-2869) (barns)	(δ , %)
0	0.5	39.00	39.23	-0.6
0	1.0	35.68	36.02	-0.9
0	1.5	32.89	33.27	-1.1
0	2.0	30.50	30.90	-1.3
0.1	0.5	37.88	37.86	0.1
0.1	1.0	33.85	33.68	0.5
0.1	1.5	30.60	30.33	0.9
0.1	2.0	27.91	27.58	1.2
0.2	0.5	36.82	36.64	0.5
0.2	1.0	32.20	31.95	0.8
0.2	1.5	28.60	28.33	1.0
0.2	2.0	25.73	25.45	1.1
0.3	0.5	35.82	35.60	0.6
0.3	1.0	30.70	30.59	0.4
0.3	1.5	26.85	26.86	0
0.3	2.0	23.87	23.95	-0.3
0.4	0.5	34.87	34.72	0.4
0.4	1.0	29.33	29.49	-0.5
0.4	1.5	25.31	25.73	-1.6
0.4	2.0	22.26	22.81	-2.4

Table 4. Resonance Integral (RI) for U^{235} Fission Products

$$Z_0 = 172.40 \text{ barns}$$

$$a_0 = 0.1506$$

$$a_1 = 2.1662$$

P	F	RI (formula 3) (barns)	RI (ORNL-2869) (barns)	(δ, %)
0	0.5	160.33	161.11	-0.5
0	1.0	149.83	151.41	-1.0
0	1.5	140.63	142.65	-1.4
0	2.0	132.49	134.82	-1.7
0.1	0.5	145.66	145.38	0.2
0.1	1.0	126.10	125.70	0.3
0.1	1.5	111.17	110.95	0.2
0.1	2.0	99.40	99.54	-0.1
0.2	0.5	133.45	131.65	1.4
0.2	1.0	108.85	107.24	1.5
0.2	1.5	91.91	91.07	0.9
0.2	2.0	79.53	79.54	0.0
0.3	0.5	123.12	121.62	1.2
0.3	1.0	95.75	95.03	0.8
0.3	1.5	78.34	78.79	-0.6
0.3	2.0	66.28	67.74	-2.2
0.4	0.5	114.29	112.71	1.4
0.4	1.0	85.47	85.27	0.2
0.4	1.5	68.26	69.47	-1.7
0.4	2.0	56.82	59.02	-3.7

Table 5. Thermal Cross Section ($g \sigma_0$) for Pu^{239} Fission Products

$$Z_0 = 53.74 \text{ barns}$$

$$a_0 = 0.0702$$

$$a_1 = 0.9298$$

P	F	$g \sigma_0$ (formula 3) (barns)	$g \sigma_0$ (ORNL-2869) (barns)	(δ , %)
0	0.5	51.92	52.18	-0.5
0	1.0	50.21	50.70	-1.0
0	1.5	48.62	49.31	-1.4
0	2.0	47.12	47.96	-1.8
0.1	0.5	49.69	49.51	0.4
0.1	1.0	46.20	45.95	0.5
0.1	1.5	43.17	42.88	0.7
0.1	2.0	40.52	40.26	0.6
0.2	0.5	47.64	47.19	1.0
0.2	1.0	42.78	42.34	1.0
0.2	1.5	38.82	38.58	0.6
0.2	2.0	35.54	35.52	0.1
0.3	0.5	45.75	45.20	1.2
0.3	1.0	39.83	39.55	0.7
0.3	1.5	35.27	35.73	-1.3
0.3	2.0	31.64	32.24	-1.9
0.4	0.5	44.01	43.49	1.2
0.4	1.0	37.27	37.29	-0.1
0.4	1.5	32.31	32.98	-2.0
0.4	2.0	28.52	29.77	-4.1

Table 6. Resonance Integral (RI) for Pu^{239} Fission Products

$$Z_0 = 265.89 \text{ barns}$$

$$a_0 = 0.0724$$

$$a_1 = 2.490$$

P	F	RI (formula 3) (barns)	RI (ORNL-2869) (barns)	(δ , %)
0	0.5	256.60	256.80	-0.1
0	1.0	247.94	248.41	-0.2
0	1.5	239.84	240.66	-0.3
0	2.0	232.26	233.49	-0.5
0.1	0.5	229.08	229.32	-0.1
0.1	1.0	201.22	201.17	0
0.1	1.5	179.40	179.09	0.2
0.1	2.0	161.85	161.41	0.3
0.2	0.5	206.89	206.87	0
0.2	1.0	169.31	168.82	0.3
0.2	1.5	143.29	142.73	0.4
0.2	2.0	124.20	123.92	0.2
0.3	0.5	188.61	188.36	0.1
0.3	1.0	146.14	145.57	0.4
0.3	1.5	119.28	119.10	0.2
0.3	2.0	100.76	101.19	-0.4
0.4	0.5	173.30	172.90	0.2
0.4	1.0	128.55	128.18	0.3
0.4	1.5	102.16	102.50	-0.3
0.4	2.0	84.76	85.83	-1.2

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Fig. 1. Macroscopic fission Product Core Section vs. Cycle time (Normalized Units)

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