rather than the reactivity feedback. Thus, for the case where both the heat capacity and the temperature coefficient are temperature dependent, the temperature at the end of the excursion can be either greater or less than for the constant slope case, depending upon the details of the temperature-dependent quantitites.

Another point which can be inferred from Fig. 2 is that when the slope of $g(E)$ is not constant, multiplication of $g(E)$ by a constant will change not only the energy release but also the reactivity feedback at the termination of the excursion. Furthermore, for a given $g(E)$, the ratio of the reactivity feedback to δk_p at the termination of the excursion depends upon δk_p itself. This contrasts with the case of constant slope discussed above.

Consider now the peak power reached during the excursion. Equation (3) can be rewritten in the form $1(P - P_0) = \delta k_p \int dE - \int g(E) dE$ or $P - P_0 = \int \frac{(\delta k_p - g(E))}{\ell} dE$. This result can be stated in the form of a second lemma: "The increase of reactor power from the start of the excursion is proportional to the energy integral of the prompt reactivity. The constant of proportionality is the inverse of the prompt-neutron lifetime." The validity of this lemma rests on the same assumptions as for the first lemma.

The peak power will be reached when $g(E) = \delta k_p$. Thus, we see from the second lemma that in Fig. 2 the peak power will be proportional to the shaded area to the left of the intersection of the $g(E)$ curve and the δk_p line. From Fig. 2 it can be seen that peak power is greater than would be the case if the $g(E)$ curve retained its initial slope. On the other hand the peak power is less than would be predicted if one used the average slope of $g(E)$ up to the point where $g(E) = \delta k_p$.

In the constant slope case, one can immediately conclude from Fig. 1 that the peak power is proportional to the square of the initial reactivity insertion δk_p. Also, one can deduce that the peak power is inversely proportional to the temperature coefficient. No such simple relationships exist for the general case of non-constant slope.

It is sometimes helpful to extend simple theories by defining appropriate 'average' or 'effective' values for important parameters. However, an important conclusion from the figures and discussion above is that it is not generally possible to choose an average (constant) slope for $g(E)$ which will correctly give both the energy release at the 'termination' of the excursion and peak power during the excursion. (By choosing a constant slope one, of course, immediately precludes the possibility of correctly obtaining the reactivity feedback at the 'termination' of the excursion.) Thus, the simple Nordheim-Fuchs' model should be approached with caution if either the heat capacity or the temperature coefficient varies significantly with temperature. One should use similar caution with more elaborate models which include heat transfer and delayed-neutron effects but ignore the temperature dependence of the important parameters.

B. Wolfe

General Electric Company
Atomic Power Equipment Department
San Jose, California

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A Simple Method of Fitting SOFOCATE Thermal Constants for Highly Enriched Water Moderated Reactors

In some applications, such as core depletion studies, detailed thermal spectrum calculations cannot be performed for each case, owing to the large number of cases involved. Consequently a very simple spectrum model such as the Maxwellian has usually been used, which leads to errors that are not entirely mutually compensating. The SOFOCATE[1] model is a more accurate representation of the thermal spectrum, and Calame *et al.*[2], have described a variational technique for obtaining fitted SOFOCATE constants for use in depletion studies. This note describes an alternative and simpler method of comparable accuracy, which enables fitted SOFOCATE constants to be obtained by hand calculation, or with very small expenditure of computer time.

The scheme is based on the fact that for hydrogen moderated mixtures with approximately $1/v$ absorption, the SOFOCATE spectrum, and hence the spectrum average of any cross-section, is a function of only two variables, the moderator temperature and the ratio of 2200 m/s macroscopic absorption cross-section to the hydrogen number density.

It is found that any cross-section without a pronounced resonance peak in the thermal group may

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[1] H. AMSTER and R. SUAREZ, "The Calculation of Thermal Constants Averaged over a Wigner-Wilkins Flux Spectrum: Description of the SOFOCATE Code." WAPD-TM-39 (1957).

[2] G. P. CALAME, *et al.*, "A Two-Mode Variational Procedure for Calculating Thermal Diffusion Theory Parameters," *Nucl. Sci. Eng.* 10, 31-39 (May 1961).

be fitted, generally within 1%, by an expression of the form:

$$\bar{\sigma} = A_0 + A_1\theta + \frac{B_0 + B_1\theta}{C_0 + C_1\theta + (a/H)}$$

where

$\bar{\sigma}$	is the fitted SOFOCATE average microscopic cross-section
A_0, A_1, etc.	are fitting constants
θ	is the moderator temperature
(a/H)	is the spectrum hardening factor defined by:

$$(a/H) = 1/N_H \sum_i N_i \, \sigma_{aoi}$$

N_i	is the number density of element i,
σ_{aoi}	is the 2200 m/s absorption cross-section of element i.

The macroscopic cross-sections for a homogeneous mixture may be obtained from the average microscopic cross-sections in the usual way, e.g.

$$\Sigma_a = \sum_i N_i \, \bar{\sigma}_{ai} \; .$$

The SOFOCATE D cannot be fitted accurately by the use of a fit to the average hydrogen transport cross-section printed out by SOFOCATE, since SOFOCATE computes D by averaging $D(E)$ over the spectrum, rather than averaging $\Sigma_{tr}(E)$. An accurate fit to D may be obtained by defining an effective hydrogen transport cross-section, $\hat{\sigma}_{trH}$, in terms of the SOFOCATE values of D and Σ_a and the (energy independent) values of $(1 - \bar{\mu})\sigma_s$ for all the other elements in the mixture, and obtaining a fit to $\hat{\sigma}_{trH}$.

$\hat{\sigma}_{trH}$ is defined by the equation:

$$D_{\text{SOF}} = \frac{1/3}{N_H \, \hat{\sigma}_{trH} + \Sigma_{a\text{SOF}} + \sum_{i \neq H} N_i[(1 - \bar{\mu})\sigma_s]_i} \tag{1}$$

and has no direct physical significance. It is found that $\hat{\sigma}_{trH}$ may be fitted by an expression of the form:

$$\hat{\sigma}_{trH} = A_0 + A_1\theta + \frac{B_0 + B_1\theta}{C_0 + C_1\theta + (a/H)} + (F_0 + F_1\theta)(x/H)$$

where (x/H) is defined by:

$$(x/H) = 1/N_H \sum_{i \neq H} N_i \, [(1 - \bar{\mu})\sigma_s]_i$$

and F_0 and F_1 are fitting constants.

The fitted D is then obtained by substituting the fitted values of Σ_a and $\hat{\sigma}_{trH}$ into Eq. 1.

Fitting constants for a unit $1/v$ cross-section, and some non-$1/v$ cross-sections frequently encountered during the analysis of highly enriched water moderated cores are given in Table I. These constants are consistent with the Rolls-Royce and Associates SOFOCATE library SPL1, which is based on Amster's 2nd deck[3], with modifications where more recent data are available.

The accuracy of the fitting scheme is demonstrated in Table II, in which SOFOCATE and fitted constants are compared for the mixtures of Ref. 2. It may be seen that the errors are generally less than 1%.

The range of validity of the fitting constants of Table I is:

$$0 \leq \theta \leq 300 \text{ C}$$

$$0 \leq (a/H) \leq 12 \text{ barns/H atom}$$

$$0 \leq (x/H) \leq 12 \text{ barns/H atom.}$$

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[3] H. AMSTER, "Cross-sections in the SOFOCATE Code, Second Deck." WAPD-TM-67, (1957).

TABLE I

Thermal Fitting Constants[a, b]

Element and cross-section	σ_{ao}	$(1 - \bar{\mu})\sigma_s$	A_0	A_1	B_0	B_1	C_0	C_1	F_0	F_1
H transport	3320 0	0	7562 1	-1634 -2	1128 3	1497 0	4700 1	2165 -1	1800 0	-2000 -3
unit $1/v$	1000 1	0	3159 0	-4272 -4	5416 1	-7034 -3	9012 1	2238 -1	-	-
U^{235} absorption	6790 3	1496 2	1841 3	-2064 -1	3778 4	-8535 0	8846 1	2288 -1	-	-
U^{235} fission	6790 3	1496 2	1552 3	-1771 -1	3276 4	-7821 0	8882 1	2253 -1	-	-
Sm^{149} absorption	4090 5	0	2011 5	-1959 2	8654 6	6823 3	1540 2	7274 -2	-	-
Xe^{135} absorption	2720 7	3000 6	5201 6	-5705 3	2620 8	1501 5	1081 2	1942 -1	-	-

[a] The numbers are written in FORTRAN E format, e.g. $-5432 \;\; 1 = -0.5432 \times 10^1$
$= -5.432$

[b] The values of A_0, A_1, etc. are consistent with temperatures expressed in degrees C.

TABLE II

Accuracy of the Fitting Scheme

Mixture	Temp. °C	Constant	SOFOCATE value	Fitted value	% error
1	20	Σ_a	5759 -1	5749 -1	-0.17
		$\nu\Sigma_f$	8947 -1	8930 -1	-0.19
		D	2241	2238	-0.13
		$\bar{\sigma}_a$ (unit $1/v$)	8076	8065	-0.14
		$\bar{\sigma}_a$ (U^{235})	5320 3	5309 3	-0.21
		$\bar{\sigma}_f$ (U^{235})	4558 3	4550 3	-0.18
		$\bar{\sigma}_a$ (Xe^{135})	2570 7	2590 7	0.78
		$\bar{\sigma}_a$ (Sm^{149})	7010 5	7120 5	1.57
1	149	Σ_a	4853 -1	4856 -1	0.06
		$\nu\Sigma_f$	7495 -1	7498 -1	0.04
		D	2503	2530	1.08
		$\bar{\sigma}_a$ (unit $1/v$)	6925	6922	-0.04
		$\bar{\sigma}_a$ (U^{235})	4456 3	4459 3	0.07
		$\bar{\sigma}_f$ (U^{235})	3819 3	3820 3	0.03
		$\bar{\sigma}_a$ (Xe^{135})	2332 7	2301 7	-1.33
		$\bar{\sigma}_a$ (Sm^{149})	7280 5	7087 5	-2.65
1	260	Σ_a	4341 -1	4335 -1	-0.14
		$\nu\Sigma_f$	6673 -1	6662 -1	-0.16
		D	2704	2714	0.37
		$\bar{\sigma}_a$ (unit $1/v$)	6255	6246	-0.14
		$\bar{\sigma}_a$ (U^{235})	3973 3	3966 3	-0.18
		$\bar{\sigma}_f$ (U^{235})	3400 3	3395 3	-0.15
		$\bar{\sigma}_a$ (Xe^{135})	2103 7	2103 7	0
		$\bar{\sigma}_a$ (Sm^{149})	7014 5	7042 5	0.40
2	20	Σ_a	7562 -1	7546 -1	-0.21
		$\nu\Sigma_f$	1344	1341	-0.22
		D	3411	3440	0.85
		$\bar{\sigma}_a$ (unit $1/v$)	7369	7356	-0.18
		$\bar{\sigma}_a$ (U^{235})	4813 3	4802 3	-0.23
		$\bar{\sigma}_f$ (U^{235})	4121 3	4112 3	-0.22
		$\bar{\sigma}_a$ (Xe^{135})	2314 7	2326 7	0.52
		$\bar{\sigma}_a$ (Sm^{149})	6546 5	6616 5	1.07

TABLE II (Continued)

Mixture	Temp. °C	Constant	SOFOCATE value	Fitted value	% error
2	149	Σ_a	6539 -1	6533 -1	-0.09
		$\nu\Sigma_f$	1158	1157	-0.09
		D	3671	3722	1.39
		$\bar{\sigma}_a$ (unit 1/v)	6485	6472	-0.20
		$\bar{\sigma}_a$ (U^{235})	4149 3	4145 3	-0.10
		$\bar{\sigma}_f$ (U^{235})	3552 3	3548 3	-0.11
		$\bar{\sigma}_a$ (Xe^{135})	2133 7	2099 7	-1.59
		$\bar{\sigma}_a$ (Sm^{149})	6778 5	6587 5	-2.82
2	260	Σ_a	5930 -1	5912 -1	-0.30
		$\nu\Sigma_f$	1047	1044	-0.29
		D	3883	3914	0.80
		$\bar{\sigma}_a$ (unit 1/v)	5939	5921	-0.30
		$\bar{\sigma}_a$ (U^{235})	3756 3	3744 3	-0.32
		$\bar{\sigma}_f$ (U^{235})	3212 3	3201 3	-0.34
		$\bar{\sigma}_a$ (Xe^{135})	1944 7	1936 7	-0.41
		$\bar{\sigma}_a$ (Sm^{149})	6553 5	6545 5	-0.12
3	20	Σ_a	1924 -1	1921 -1	-0.16
		$\nu\Sigma_f$	0	0	0
		D	1608	1592	-1.00
		$\bar{\sigma}_a$ (unit 1/v)	8682	8667	-0.17
		$\bar{\sigma}_a$ (U^{235})	5755 3	5741 3	-0.24
		$\bar{\sigma}_f$ (U^{235})	4933 3	4922 3	-0.22
		$\bar{\sigma}_a$ (Xe^{135})	2783 7	2806 7	0.83
		$\bar{\sigma}_a$ (Sm^{149})	7378 5	7508 5	1.76
3	149	Σ_a	1613 -1	1614 -1	0.06
		$\nu\Sigma_f$	0	0	0
		D	1888	1904	0.85
		$\bar{\sigma}_a$ (unit 1/v)	7279	7284	0.07
		$\bar{\sigma}_a$ (U^{235})	4703 3	4711 3	0.17
		$\bar{\sigma}_f$ (U^{235})	4033 3	4039 3	0.15
		$\bar{\sigma}_a$ (Xe^{135})	2489 7	2461 7	-1.12
		$\bar{\sigma}_a$ (Sm^{149})	7669 5	7470 5	-2.59

TABLE II (Continued)

Mixture	Temp. °C	Constant	SOFOCATE value	Fitted value	% error
3	260	Σ_a	1440 -1	1440 -1	0
		$\nu\Sigma_f$	0	0	0
		D	2096	2094	-0.09
		$\bar{\sigma}_a$ (unit $1/v$)	6500	6499	-0.02
		$\bar{\sigma}_a$ (U^{235})	4140 3	4139 3	-0.02
		$\bar{\sigma}_f$ (U^{235})	3546 3	3545 3	-0.03
		$\bar{\sigma}_a$ (Xe^{135})	2225 7	2231 7	0.27
		σ_a (Sm^{149})	7362 5	7419 5	0.77

U^{235} absorption does not depart sufficiently from $1/v$ behavior to affect the accuracy significantly. However, the method is not directly applicable to mixtures containing large quantities of Pu.

The computer time required to find the thermal constants of a typical mixture containing 6 elements is very small—much less than 0.01 sec. IBM-7090 time. This may be compared with typical values of 0.25 sec and 17 sec. IBM-704 time respectively for SPG and SOFOCATE, quoted in Ref. 2.

In some studies, only a few particular temperatures are of interest. In this case improved accuracy in fitting non-$1/v$ cross-sections as Sm^{149} and Xe^{135} absorption may be obtained by simplifying the fitting equations to the form:

$$\bar{\sigma} = A + \frac{B}{C + (a/H)}$$

and fitting A, B and C to SOFOCATE results at each of the temperatures of interest. This simplification also leads to a considerable reduction in computing time.

There is no physical significance attached to the form of the fitting equations, which are merely an empirical fit to a series of SOFOCATE results.

K. R. Teare

Rolls-Royce and Associates Limited
P. O. Box 31
Derby, England

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