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MULTIGROUP CALCULATIONS OF RESONANCE NEUTRON CAPTURE IN A THICK SLAB OF DEPLETED URANIUM

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SUMMARY

A recent experiment and calculation performed for a layered shield-like assembly of a 3.14-centimeter-thick depleted-uranium slab, sandwiched between a pair of polyethylene slabs, verified a multigroup cross-section calculation procedure, GAROL, and an accompanying detailed multigroup discrete-ordinates transport calculation. The experiment and 10-group calculation concentrated on the energy region from 3 to 11 eV containing the large 6.68-eV resonance in uranium-238 (U^{238}). The present work examines several widely used group-averaged cross-section formulations as they would be applied over the 3- to 11-eV energy interval; the integral and spatial capture rates and capture gamma leakage rates as calculated for the experimental geometry with various one-group cross-section formulations are compared with the multigroup, experimentally verified, transport calculation to determine the validity of these one-group formulations.

When the 3- to 11-eV one-group-averaged cross section obtained from GAROL is used in a one-group transport calculation, the total neutron capture rate is preserved but the correct spatial distribution is not. This incorrect spatial distribution results in an underestimate by 20 percent of capture gamma leakage from the uranium slab because of the gamma ray attenuation.

One-group cross sections obtained from results of transport calculations using GAM-II provided cross sections that did not preserve the total neutron capture rate and were incapable of predicting the correct spatial distribution of captures. The errors in total capture rate combined with the calculated incorrect spatial distribution to result in gamma leakage rates ranging from 1 to 60 percent too low. However, the good agreement in some cases was fortuitous and is not generally predictable.

Of the methods examined, the greatest confidence is placed in the GAROL-generated-group cross section because it at least preserved the total neutron capture rate. The resultant error in gamma leakage rate because of the incorrect spatial distribution of captures may be acceptable for shielding calculations. Furthermore because the GAROL cal-

culation obviates the separate multigroup transport calculation to obtain a group cross section, it represents a convenient method of calculating broad-group cross sections for resonance absorbers.

INTRODUCTION

A man-rated optimum shield for a compact reactor is generally composed of alternate layers of hydrogenous, lightweight neutron shielding material and high-atomic-number, heavy-weight gamma-shielding material. Because the gamma-shielding material absorbs neutrons and produces capture gammas, a calculation of the spatial distribution of neutron capture rate is necessary to determine the dose from these capture gammas. Optimum placement of the gamma-shielding material relative to the neutron shielding, and hence the shield weight, is dependent on accurate calculation of these secondary sources.

A large fraction of neutron captures in the gamma shielding material is in the so-called resolved resonance region, extending from about 1 eV to 1 keV. In this region, the cross section is characterized by very high but narrow resonance cross sections. The question of how to handle the rapidly varying cross sections in terms of a broad multigroup structure (i.e., much broader than the width of the resonance) for use in subsequent diffusion or transport calculations has been answered for the case of small resonance-absorber lumps by the method of Nordheim (refs. 1 and 2). The applicability of the method has not been tested for absorbers of the thicknesses (2 to 10 cm) expected in high-performance compact reactor shields.

A recent experiment (ref. 3) employing the time-of-flight method, measured the neutron energy spectra from about 1 eV to 1 keV at several positions in a 3.14-centimeter-thick slab of depleted uranium (0.23 percent uranium-235 (U^{235}), the remainder U^{238}) that was sandwiched between two slabs of borated polyethylene, each 2.49 centimeters thick. The experiment approximates a layered shield configuration. The energy spectrum of neutrons traveling in a direction normal to the slab array was calculated using a one-dimensional discrete-ordinates transport code for comparison with the measurements. The calculation that is used as a reference was made in the 3- to 11-eV energy interval using a 10-energy-group cross-section set generated by the code GAROL (ref. 4). The 3- to 11-eV interval contains one narrow resonance centered at 6.68 eV with a peak value of about 4000 barns. The 10-group energy split selected permits a good representation of the cross-section variation. The good agreement with experiment reported in reference 3 verified GAROL as a means of generating fine-group cross sections and the one-dimensional discrete-ordinates multigroup method as a means of calculating neutron transport.

The shield designer, trying to perform a neutron transport calculation over the complete energy range of interest, from 0 to 15 MeV, cannot afford the luxury of 10 energy groups about each resonance; one energy group in an interval as 3 to 11 eV is a more reasonable goal. In this report, the fine-group transport calculation of reference 3 is repeated to determine the spatial distribution of 3- to 11-eV neutrons captured in U^{238} for the experimental configuration. This is used as a standard for comparison with the capture distribution as calculated by one-group transport calculations, where the one-group cross section, typical of a group cross section used in a multigroup calculation, is generated by several methods currently available using the codes GAROL and GAM-II (ref. 5). Furthermore, the relative gamma leakage rates, which depend on both the total number of captures and the spatial distribution of captures, are compared to determine the ultimate effect of the use of various one-group formulations.

3- TO 11-eV NEUTRON CAPTURE RATE IN URANIUM-238

A reference capture rate was obtained for later comparison by duplicating the 10-group 3- to 11-eV neutron transport calculation of reference 3 with the addition of the calculation of neutron capture rate. Because of the experimental verification of the calculation methods, this capture rate is regarded as an accurate one. The experimental geometry is represented by the slab array shown in figure 1. Atom densities for each region are listed in table I. (Minor differences between the data used in this work and ref. 3 may exist, but their use will not affect the conclusions.)

A GAROL calculation of region-averaged flux was made for each region of the cell of figure 1 using 770 points equally spaced in the energy interval of 3.3 to 11.0 eV. Reso-

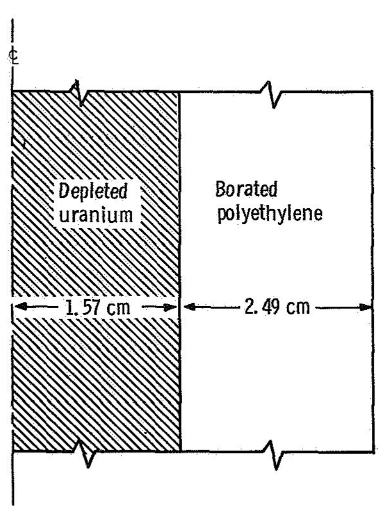


Figure 1. - Analytic mockup of experiment.

TABLE I. - ATOM DENSITIES

Region	Isotope	atoms/cm^3
Depleted uranium	U^{235}	0.0001074×10^{24}
	U^{238}	.04202
Polyethylene	H	.070
	C	.035
	B^{10}	.00258

nance parameters for U^{238} and U^{235} were taken from reference 6 and Doppler broadened corresponding to a temperature of 300 K. Group cross sections were calculated by GAROL within a region using equations (1):

$$\bar{\sigma}_a = \frac{\int \bar{\varphi}(E)\sigma_a(E)dE}{\int \bar{\varphi}(E)dE} \tag{1a}$$

$$\bar{\sigma}_s = \frac{\int \bar{\varphi}(E)\sigma_s(E)dE}{\int \bar{\varphi}(E)dE} \tag{1b}$$

where

$\bar{\varphi}(E)$ appropriate (absorber- or moderator-) region-average neutron energy flux calculated by GAROL $\bar{\varphi}(E) \sim \int \varphi(E, r)d^3r$

$\sigma_a(E)$ absorption cross section

$\sigma_s(E)$ scattering cross section

and the integrations are made over an energy range of interest. The group cross sections calculated and energy group split used are listed in table II. The total cross section is

TABLE II. - GAROL ENERGY GROUP SPLIT

Group	Energy, eV	Calculated cross section, b	
		Absorption, σ_a	Scattering, σ_s
1	11.0 to 9.0	0.52	13.42
2	9.0 to 7.6	1.57	14.78
3	7.6 to 7.2	7.12	17.57
4	7.2 to 6.99	21.18	21.67
5	6.99 to 6.76	91.85	32.88
6	6.76 to 6.6	3519.17	232.79
7	6.6 to 6.1	35.39	5.65
8	6.1 to 5.8	8.03	8.26
9	5.8 to 4.5	2.09	10.35
10	4.5 to 3.3	.68	11.30

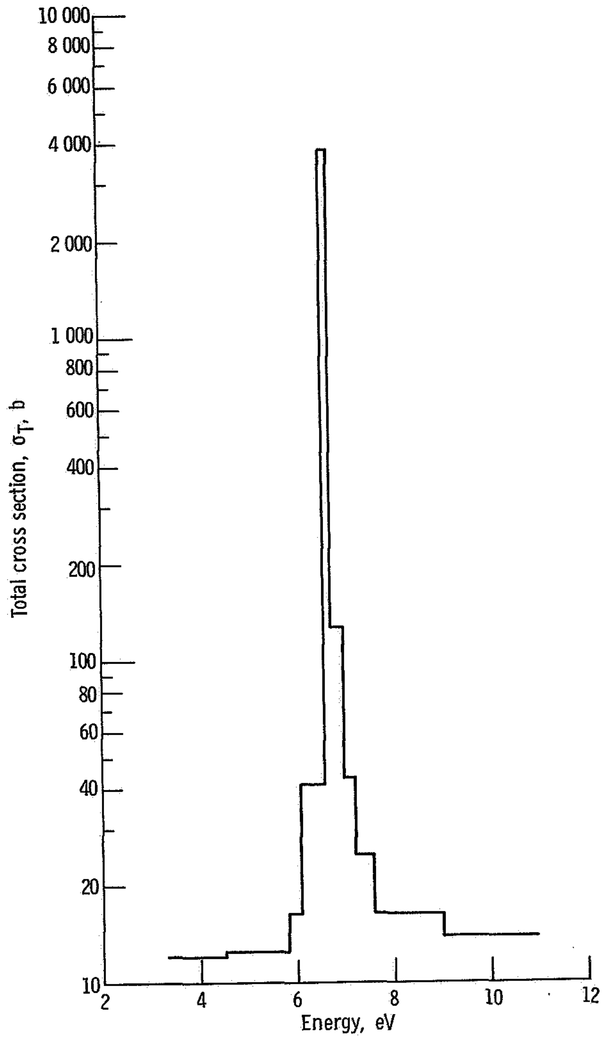


Figure 2. - Uranium-238 total cross section from 10-group-GAROL calculation.

plotted in figure 2; this choice of energy group split preserves much of the cross-section detail.

A 10-energy-group transport calculation was made for the geometry of figure 1 using the discrete-ordinates transport code ANISN (ref. 7). The uranium capture and scatter cross sections of table II were used in this calculation; a scatter with uranium was assumed to keep the neutron within the same energy group. A hand-calculated set of down-scatter cross sections for the moderator elements was used because GAROL does not calculate a down-scatter cross section. In the depleted uranium region, 314 mesh intervals each 0.005 centimeter wide were used; in the polyethylene, 20 intervals were used. A P_0 scattering approximation and a six-point full-range Gauss-Legendre angular quadrature set were used. The source was assumed to be in the polyethylene only, flat in spatial

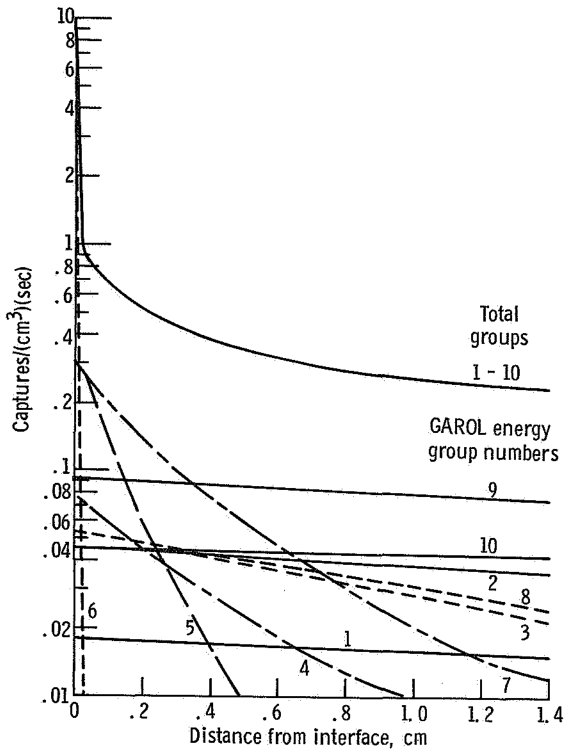


Figure 3. - Relative 3- to 11-eV neutron capture rate in uranium-238 by energy group. 10-Group ANISN calculation with GAROL cross sections.

TABLE III. - TOTAL CAPTURES IN URANIUM-238 BY GROUP

[10-Group GAROL calculation.]

Group	Captures
1	1.203×10^{-3}
2	2.835
3	2.006
4	1.404
5	1.670
6	1.321
7	4.003
8	2.093
9	5.437
10	2.924
Sum	2.490×10^{-2}

distribution, isotropic, and proportional to 1/E in energy.

The capture rate of 3- to 11-eV neutrons in the U^{238} of the depleted uranium is shown in figure 3 as a function of distance from the interface. The capture rate is dominated at the interface by captures in group 6 containing the peak of the 6.68-eV resonance. The capture rate decreases by about a decade in the first 0.02 centimeter, is dominated by captures in the resonance wings (groups 5 and 7) in the next 0.2 centimeter, and is finally determined by captures in the flats between resonances (groups 1, 2, 3, 8, 9, and 10). The total capture rate in U^{238} for the region is listed, by energy group, in table III.

ONE-GROUP CROSS SECTION FOR THE 3- TO 11-eV INTERVAL

There are several ways to generate a group cross section. The present report considers two spatially averaged formulations. A spatially averaged group cross section is, in principle, obtained using an equation such as equation (2)

$$\overline{\sigma} = \frac{\int \varphi(E, r)\sigma(E)d^3r\ dE}{\int \varphi(E, r)d^3r\ dE} \tag{2}$$

where the integrals are performed over the spatial region and energy range of interest. The present report considers a group cross section for the 3- to 11-eV energy interval generated by the following analogs of equation (2). The first is

$$\overline{\sigma} = \frac{\int \overline{\varphi}(E)\sigma(E)dE}{\int \overline{\varphi}(E)dE} \tag{3}$$

where $\overline{\varphi}(E)$ is the region-average flux calculated by GAROL $\varphi(E) \sim \int \varphi(E, r)d^3r$. The second is the multigroup equivalent of equation (2)

$$\overline{\sigma} = \frac{\sum\sum \varphi_{ij}\sigma_i\ \Delta V_j}{\sum\sum \varphi_{ij}\ \Delta V_j} \tag{4}$$

where φ_{ij} is the multigroup flux for the i^{th} energy and j^{th} spatial interval (of volume V_j), and σ_i is a fine-group cross section. The flux φ_{ij} is obtained from a fine multigroup transport calculation performed on, for example, a simple, representative slab geometry to obtain a $\overline{\sigma}$ for later use in a more geometrically detailed one-dimensional or two-dimensional transport calculation. Values of fine-group cross section σ_i considered in the present report are those generated by GAROL and GAM-II; the GAM-II fine-group cross sections presently considered are those 1/E-weighted (from the GAM-II library tape) and those calculated using the spatially dependent mode of the Nordheim method as coded in GAM-II.

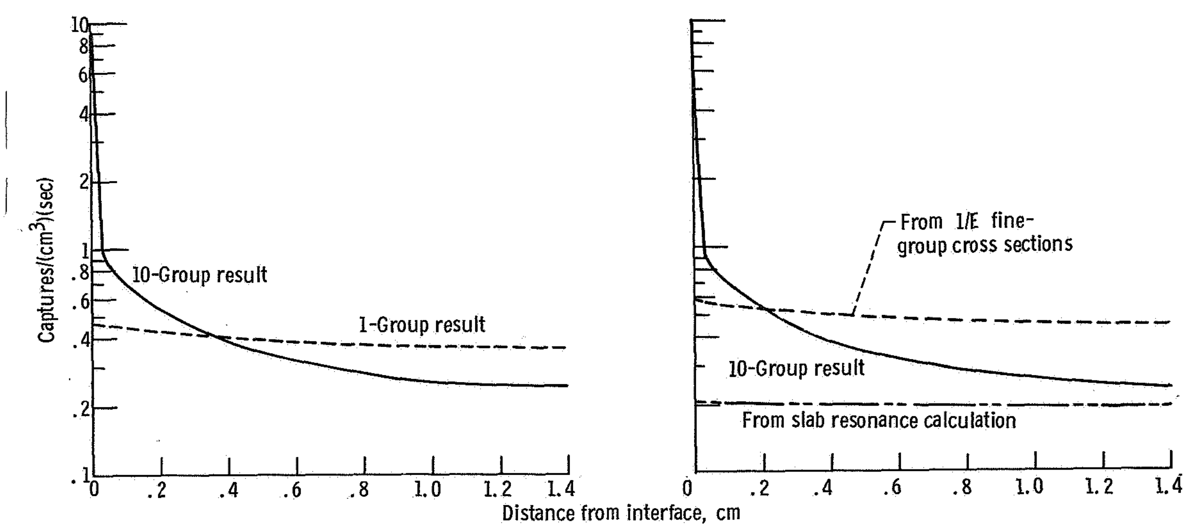
One-group discrete-ordinates transport calculations were performed with each of the one-group cross sections obtained for the 3- to 11-eV intervals; except for the energy group structure, the calculations were performed as indicated in the section 3- to 11-eV NEUTRON CAPTURE RATE IN URANIUM-238. Several figures of merit were obtained for comparison with the accurate 10-group result. These are total capture rate, spatial distribution of captures, and the relative capture gamma leakage from the slab. The latter is calculated from the capture distribution using simple point kernel methods.

RESULTS OF ONE-GROUP TRANSPORT CALCULATIONS

Results with GAROL-Generated Cross Sections

Cross section. - The GAROL code calculated a capture cross section of 2.23 barns for the 3.3- to 11-eV energy interval using equation (3). From the results of the discrete-ordinates transport calculation performed with the 10 energy groups of table II, a capture cross section of 2.24 barns was obtained for the 3.3- to 11-eV energy interval using equation (4). Reference 3 commented on the good agreement (7 percent) in the volume-flux integral as calculated by GAROL and that calculated in the 10-group discrete-ordinates calculation. This agreement might be extended to cite the good agreement in capture cross section as calculated by GAROL (using eq. (3)) and the discrete-ordinates transport code (using eq. (4)). This good agreement demonstrates the utility of GAROL for obtaining accurate broad-group spatially weighted cross sections, obviating the multigroup-transport calculation.

Transport calculation. - The relative neutron capture rate in U^{238} calculated with the one-group GAROL cross section is plotted in figure 4(a) as a function of the distance from the U^{238}-polyethylene interface. The corresponding 10-group result is also plotted for comparison. The total number of captures and relative gamma leakage (in terms of dose) is listed in table IV (case 2). The use of the spatial-flux-weighted cross section has preserved the total capture rate. But, even though the total neutron capture rate is preserved, the difference in spatial distribution of captures results in a gamma dose which is low by 19 percent.



(a) Capture rate calculated using one-group GAROL cross section.

(b) Capture rate calculated using one-group spatially weighted GAM-II fine-group cross sections.

Figure 4. - Relative 3- to 11-eV neutron capture rate in uranium-238.

TABLE IV. - RESULTS OF ONE-GROUP TRANSPORT CALCULATIONS

Cross section used in one-group calculation	Case number	Total number of captures in U^{238}	Relative capture gamma dose at polyethylene surface
Results of 10-group calculation made with GAROL-calculated cross-sections, listed for reference	1	0.02490	1.000
One-group GAROL-calculated cross section	2	0.02578	0.814
One-group cross section calculated from results of five-group transport calculation made with the following GAM-II cross sections:			
1/E flux-weighted values	3	0.03105	0.990
Calculated for discrete U^{238} slab	4	.01280	.400

Results with Spatially Weighted GAM-II Cross Sections

Cross sections. - The cross-section library (and fine-group cross section averaging routines of Nordheim) of GAM-II is now considered as a source of fine-group cross sections to obtain a spatially weighted group cross section from equation (4). GAM-II uses a constant energy group width of 0.25 lethargy units in the resolved resonance region; hence the flexibility of a fine-group split such as used in the 10-group GAROL calculation (e.g., see fig. 2) is not available. Five of the GAM-II fine groups fit in the 3- to 11-eV energy interval presently considered.

Several choices of GAM-II fine-group cross sections are available for the 0.25-lethargy-unit-group split. Two cases are presently considered. The first is the 1/E weighted case; that is,

$$\sigma_i = \frac{\int (1/E)\sigma(E)dE}{\int \frac{dE}{E}} \tag{5}$$

The second case uses the method of Nordheim to calculate the total capture rate and a fine-group averaged cross section σ_i. GAM-II is coded to calculate a fine-group capture cross section σ_i from equation (6):

$$\sigma_i = \frac{\int \overline{\varphi}(E)\sigma(E)dE}{\Delta u} \tag{6}$$

(Only 1/E-weighted fine-group scatter cross sections are available in GAM-II.) A comparison of equation (6) with equation (3), the GAROL formulation, shows that the numerators (and the method used to calculate collision density) of both equations are the same; the denominators are not. The fomulation of equation (6) tacitly assumes that the σ_i calculated is to be used only in a 1/E flux; this is, of course, not the case within a lump of absorber. Nevertheless, values of σ_i were generated using the GAM-II Nordheim method to determine the consequence of their use. These were generated for the case of a 3.14-centimeter slab of depleted uranium with no moderator in the absorber (1/E flux in exterior moderator region is always assumed in a GAM-II Nordheim calculation). This case has essentially the same geometric configuration as that used in the GAROL calculation and would give the same σ_i as a GAROL calculation (for the same energy boundaries) if equation (3) was used instead of equation (6).

The one-group capture cross section calculated by equation (4) from the results of a five-group transport calculation with each of the three GAM-II cross section sets is listed in table V. (Some results of the five-group transport calculation appear in the appendix.) The use of equation (6) by GAM-II instead of equation (3) results in a set of σ_i, for the case of a 3.14-centimeter slab of U^{238}, which is consistently too low; the value of $\overline{\sigma}$ of 0.92 barn obtained from results of the five-group transport calculation and equation (4) is more than a factor of 2 lower than that calculated by a comparable GAROL-generated set of σ_i.

Transport calculations. - The relative neutron capture rate in U^{238} as calculated with these two one-group spatially weighted GAM-II cross sections is plotted in figure 4(b)

TABLE V. - ONE-GROUP CAPTURE CROSS SECTION FOR 3- TO 11-eV, 3.14-CENTIMETER SLAB OF URANIUM-238

[Cross section is calculated from results of a fine-group transport calculation for the 3.14-cm slab of U^{238} in polyethylene.]

Cross sections used in fine-group transport calculation	One-group capture cross section in 3- to 11-eV interval for 3.14-cm slab of U^{238}, b
10-Group GAROL-calculated values	2.24
GAM-II 1/E flux-weighted values	3.20
GAM-II-calculated values for a discrete 3.14-cm slab of U^{238}	.92

as a function of distance from the U^{238} - polyethylene interface. The 10-group GAROL result is also plotted for comparison. The total number of captures and relative gamma leakage rate are listed in table IV as cases 3 and 4. In case 3, overestimates in total neutron capture rate make up for differences in the spatial distribution of captures and result in near-correct gamma leakage rates. Again, whether or not this is generally true cannot be estimated from this study. The differences in formulation of group capture cross section result in case 4 being a factor of 2 too low in neutron capture rate and $2\frac{1}{2}$ too low in gamma leakage rate instead of giving the same results as case 2.

CONCLUDING REMARKS

Although this study has been confined to a single, 3.14-centimeter thickness of resonance absorber, and a single energy region extending from 3 to 11 eV containing only one large resonance, insight has been gained to make recommendations regarding calculation of multigroup cross sections in the resolved resonance region for thick absorbers. From the detailed 10-group spatial calculation, an accurate reference for comparison was established. Comparison of one-group-averaged cross sections for the 3- to 11-eV interval as calculated by the code GAROL and calculated from results of a detailed 10-group spatial calculation confirmed the GAROL method of calculating proper broad-group-region weighted-average cross sections. The use of GAROL therefore obviates a separate transport calculation of a group average cross section. Comparison of neutron capture rate, as calculated using the GAROL-averaged one-group cross section, with that calculated using the 10-group cross-section set revealed that the total neutron capture rate in U^{238} was preserved, but the spatial distribution was not. This manifested itself in a 20-percent underestimate in gamma leakage.

Capture rates calculated using one-group spatially weighted GAM-II fine-group cross sections preserved neither total capture rate nor spatial distribution of captures; results ranged from overestimates of total capture rate by 25 percent to underestimates of 50 percent depending on the choice of 1/E-weighted or Nordheim-method-weighted values. The differences in total capture rate combined with differences in spatial distribution to result in a gamma leakage rate ranging from 1 to 60 percent low. However, the good agreement is not generally predictable.

Because it preserves the total neutron capture rate, most confidence is placed in the GAROL-generated-group cross section. Furthermore, because the GAROL calculation obviates the separate transport calculation, it also represents the more convenient method of calculating broad-group cross sections for resonance absorbers.

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APPENDIX - 3- TO 11-eV NEUTRON CAPTURE RATE CALCULATED WITH GAM-II-GENERATED FIVE-GROUP CROSS-SECTION SETS

The results of the five-group transport calculations performed with GAM-II-generated fine-group cross sections used to obtain the one-group spatially weighted cross section are presented in this appendix. The fine-group cross sections considered are 1/E weighted and those calculated by the Nordheim method as coded in GAM-II for the case of the 3.14-centimeter slab of depleted uranium. The 3- to 11-eV neutron capture rate calculated with each of these five-group sets is plotted in figure 5 as a function of distance from the U^{238}-polyethylene interface. The 10-group GAROL result is shown for comparison. The total neutron capture rate and gamma leakage rate for these cases is listed in table VI.

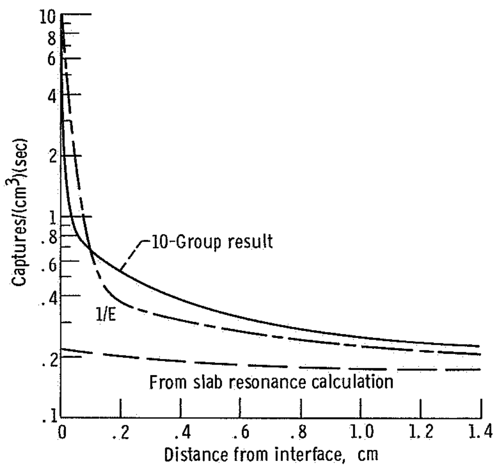

Figure 5. - Relative 3- to 11-eV neutron capture rate in uranium-238. Capture rate calculated using five-group cross sections generated by GAM-II.

TABLE VI. - 3- TO 11-eV NEUTRON CAPTURE RATE AND CAPTURE GAMMA LEAKAGE RATE CALCULATED USING GAM-II FIVE-GROUP CROSS-SECTION SETS

Cross-section set used	Total number of captures	Relative Gamma leakage rate
10-Group GAROL set (shown for reference)	0.02490	1.00
GAM-II five-Group set; 1/E weighted	.02959	1.49
Resonance calculation; 3.14-cm slab of depleted uranium	.01249	.46

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15. Supplementary Notes

16. Abstract

Capture rates were calculated, using various widely used group cross-section-generating techniques, for the case of 3 to 11 eV neutrons in a 3.14-cm-thick slab of depleted uranium sandwiched between polyethylene slabs. An experimentally verified fine-group cross-section-generating procedure, GAROL, and multigroup neutron-transport calculations for the 3- to 11-eV region provided the standard spatial capture distribution for comparison. The one-group cross section calculated by GAROL preserves the total neutron capture rate. Other one-group formulations such as obtained with GAM-II are inappropriate for use in a transport calculation in a resonance absorber and can result in a factor of 2 underestimate in neutron capture rate.

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