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UNDERSTANDING RESONANCE SELF-SHIELDING EFFECTS
WITH THE HELP OF A SIMPLIFIED CROSS-SECTION MODEL

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UNDERSTANDING RESONANCE SELF-SHIELDING EFFECTS
WITH THE HELP OF A SIMPLIFIED CROSS-SECTION MODEL*

Recent TART Monte Carlo calculations¹ have shown discrepancies with F number measurements as well as with measurements of fission density in ²³⁵U and ²³⁹PU plates.^{2,3} We have attributed these discrepancies to the fact that the group-averaged TART cross sections cannot properly treat resonance self-shielding effects, because the width of TART groups is large compared to the width of cross-section resonances.

The purpose of this note is to explain the observed discrepancies with the help of a simplified cross-section model. The model is developed in Appendix A. Some of the results are plotted in Figs. 1 and 2.

Appendix B shows the present TART cross-section group widths superimposed on a plot of ²³⁹PU and ²³⁵U fission cross sections.⁴ We see from this that reasonable values for our simplified model might be $\sigma_2/\sigma_1 \approx 10$ to 100 and $p_2 \approx 0.25$. For these values, our Fig. 1 shows that the code would overpredict the fission density by as much as a factor of eight.

Figure 2 contains this maximum overprediction factor for the worst p_2 and x/λ_2 , as a function of σ_2/σ_1 .

It can also be seen from Fig. 1 that the code will underpredict, overpredict, or correctly predict the fission density, depending on the thickness of fissionable material previously traversed by the neutron fluence:

<u>If thickness is</u>	<u>Code prediction is</u>
1) Small compared to λ_2	Correct [†] ($R = 1$)
2) Large compared to λ_2 , but small compared to $\bar{\lambda}$	High ($R \geq 1$)

* This report was originally issued as an interdepartmental memorandum on April 26, 1972.

[†] Assuming of course, that the group averaged cross sections used by the code are based on correct microscopic cross sections.

Fig. 1. R is the factor by which the computed fission density differs from the true fission density because the group-averaged fission cross section, $\bar{\sigma}$, was used in lieu of the true fission cross sections σ_1 and σ_2 . We note that the code will always give the true fission density on the front surface of the plate. Progressing into the plate, the code will at first be too high and then, at greater depth, too low.

Fig. 2. $(R_{\text{peak}})_{\text{max}}$ is the largest value of R_{peak} for a fixed value of σ_2/σ_1 ; $(\frac{x}{\lambda_2})_{\text{max}}$ is the depth in units of λ_2 at which this maximum occurs; and $(p_2)_{\text{max}}$ is the value of $p_2 = \frac{\Delta E_2}{\Delta E}$, the relative width of the resonance, for which R_{peak} attains its maximum value. $(\frac{x}{\lambda_2})_{\text{max}}$ is independent of p_2 (see Appendix A).

3) Large compared to $\bar{\lambda}$ Low ($R < 1$).
(and therefore also
large compared to λ_2)

Here, λ_2 is mean free path based on cross section at resonance peak, and $\bar{\lambda}$ is mean free path based on group-averaged cross section.

This behavior can be understood with the help of Fig. 2.

This underprediction is almost certainly present in TART F number calculations for some of our devices that have thick layers of fissionable material.

The correct prediction on the front surface, followed by overprediction and then followed by a correct prediction, has been measured in a recent F number experiment.

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APPENDIX A
SIMPLIFIED CROSS-SECTION MODEL

A. Ratio of Computed-to-True Fissions at Any Depth

The following definitions pertain to the idealized model shown in Fig. A-1:

ΔE = energy group used in code for cross-section input.

ΔE_2 = width of resonance.

Define: $p_2 \equiv \frac{\Delta E_2}{\Delta E}$

$\sigma_2 \geq \sigma_1$.

Assume: σ is all fission.*

Spectrum incident on slab, $\left(\frac{dN}{dE}\right)_0$, is constant over ΔE
(N = number of neutrons).

Group-averaged cross section used by code $\equiv \bar{\sigma} = (1 - p_2)\sigma_1 + p_2\sigma_2$. (In the example shown in Fig. A-2: $p_2 = 0.1$, $\sigma_1 = 1$, $\sigma_2 = 10$, $\bar{\sigma} = 0.9 \times 1 + 0.1 \times 10 = 1.9$.)

The following definitions pertain to the diagram shown in Fig. A-3:

Number of fissions at depth $x \equiv f_x$.

$f_x = \frac{\phi_x}{\lambda}$.

Neutron fluence at x is $\phi_x = \phi_0 e^{-\frac{x}{\lambda}} = \left(\frac{dN}{dE}\right)_0 e^{-Cx\bar{\sigma} \Delta E}$.

$\phi_0 = \left(\frac{dN}{dE}\right)_0 \Delta E$.

$\frac{1}{\lambda} = \frac{\rho}{A} N_{Avog} \sigma \equiv C\sigma$.

Code computes } $(f_x)_{\text{code}} = C\bar{\sigma} \left(\frac{dN}{dE}\right)_0 e^{-Cx\bar{\sigma} \Delta E}$ (see footnote on this page).

True fissions = $(f_x)_{\text{true}} = \left[C(1 - p_2)\sigma_1 e^{-Cx\sigma_1 \Delta E} + Cp_2\sigma_2 e^{-Cx\sigma_2 \Delta E} \right] \left(\frac{dN}{dE}\right)_0 \Delta E$.

* A better, but more complicated, treatment would be to use $\sigma_{\text{total}} = \sigma_{\text{fiss}} + \sigma_{\text{capt}} + \dots$ to compute the neutron fluence depletion, i.e.,

$$(f_x)_{\text{code}} = C\bar{\sigma}_{\text{fiss}} \left(\frac{dN}{dE}\right)_0 e^{-Cx\bar{\sigma}_{\text{total}} \Delta E}.$$

However, the present treatment brings out the main features.

Fig. A-1. Idealized model of the fission-cross-section resonance.

Fig. A-2. This figure shows the distribution of relative fissions, $\sigma \frac{dN}{dE}$, and relative neutron fluence, $\frac{dN}{dE}$, across the neutron-energy interval ΔE corresponding to the width of the cross-section group. These are shown for three distinct depths into the fissionable material: a) a depth that is small compared to λ_2 , the mean-free path based on σ_2 ($x \ll \lambda_2$); b) a depth that is large compared to λ_2 , but small compared to $\bar{\lambda}$, the mean-free path based on $\bar{\sigma}$ ($\bar{\lambda} > x > \lambda_2$); and c) a depth that is large compared to both λ_2 and $\bar{\lambda}$ ($x > \bar{\lambda}$). For $x \ll \lambda_2$, the true and computed fissions are equal; for $\bar{\lambda} > x > \lambda_2$, the computed fissions are larger than the true fissions; for $x > \bar{\lambda}$, the computed fissions are less than the true fissions, since the code overestimates the absorption of neutron fluence at all energies within the interval ΔE . (Note that this example is based on the specific values $\sigma_2/\sigma_1 = 10$, $p_2 = 0.1$. Figure 3c, furthermore, assumes $x/\bar{\lambda} = 3$ and $x/\lambda_1 = 1.5$. Also note that the area under the $\sigma \frac{dN}{dE}$ curve is proportional to the total number of fissions within the energy group ΔE .)

Fig. A-3. Geometry of the slab of fissionable material.

$$\begin{aligned}
\frac{(f_x)_{\text{code}}}{(f_x)_{\text{true}}} &\equiv R = \frac{[(1-p_2)\sigma_1 + p_2\sigma_2] e^{-Cx[(1-p_2)\sigma_1 + p_2\sigma_2]}}{(1-p_2)\sigma_1 e^{-Cx\sigma_1} + p_2\sigma_2 e^{-Cx\sigma_2}} \\
&= \frac{\left[1 + \left(\frac{p_2}{1-p_2}\right) \frac{\sigma_2}{\sigma_1}\right] e^{-Cx p_2(\sigma_2 - \sigma_1)}}{1 + \left(\frac{p_2}{1-p_2}\right) \frac{\sigma_2}{\sigma_1} e^{-Cx(\sigma_2 - \sigma_1)}} \\
R &= \frac{\left[1 + \left(\frac{p_2}{1-p_2}\right) \frac{\sigma_2}{\sigma_1}\right] e^{-\left(\frac{x}{\lambda_2}\right) p_2 \left(1 - \frac{\sigma_1}{\sigma_2}\right)}}{1 + \left(\frac{p_2}{1-p_2}\right) \frac{\sigma_2}{\sigma_1} e^{-\left(\frac{x}{\lambda_2}\right) \left(1 - \frac{\sigma_1}{\sigma_2}\right)}} \quad (\text{A-1})
\end{aligned}$$

We note that R is a function $\left(\frac{x}{\lambda_2}, p_2, \frac{\sigma_2}{\sigma_1}\right)$

Equation (A-1) is plotted in Fig. 1 of the text, for some selected values of p_2 and $\frac{\sigma_2}{\sigma_1}$.

Limiting Cases:

1) $\frac{\sigma_2}{\sigma_1} = 1$;	arbitrary p_2 and $\frac{x}{\lambda_2}$	$\rightarrow R = 1$	} Trivial cases
2) $p_2 = 0$ or 1 ;	$\frac{\sigma_2}{\sigma_1}$ and $\frac{x}{\lambda_2}$ arbitrary	$\rightarrow R = 1$	
3) $\frac{x}{\lambda_2} \ll 1$;	$\frac{\sigma_2}{\sigma_1}$ and p_2 arbitrary	$\rightarrow R = 1$, i.e., group-averaged σ gives correct fissions on surface of plate.	

B. Depth at Which R Is Maximum

$$R = \left[(1 + A) e^{-p_2 B x} \right] \left[1 + A e^{-B x} \right]^{-1},$$

where:

$$\begin{aligned}
A &\equiv \left(\frac{p_2}{1-p_2} \right) \frac{\sigma_2}{\sigma_1} \\
B &\equiv \left(1 - \frac{\sigma_1}{\sigma_2} \right) \frac{1}{\lambda_2}
\end{aligned}$$

$$\frac{dR}{dx} = \underbrace{\frac{(1 + A) e^{-p_2 B x}}{1 + A e^{-Bx}}}_{(1)} \underbrace{\left\{ -p_2 B + \frac{AB e^{-Bx}}{1 + A e^{-Bx}} \right\}}_{(2)} = 0.$$

$$\begin{aligned} (1) = 0 \Rightarrow & \left\{ \begin{array}{l} 1 + A e^{-Bx} \rightarrow \infty; \text{ cannot be, since } Bx = \text{positive} \\ (1 + A) e^{-p_2 Bx} \rightarrow 0 \Rightarrow \end{array} \right. \left\{ \begin{array}{l} 1 + A \rightarrow 0 \Rightarrow p_2 = \frac{1}{1 - \frac{\sigma_2}{\sigma_1}}; \\ \text{cannot be, since } \begin{cases} \frac{\sigma_2}{\sigma_1} \geq 1 \\ 0 \leq p_2 \leq 1 \end{cases} \\ \text{or} \\ e^{-p_2 Bx} \rightarrow 0 \Rightarrow p_2 Bx = p_2 \left[1 - \frac{\sigma_1}{\sigma_2} \right] \frac{x}{\lambda_2} \\ = \infty \Rightarrow \frac{x}{\lambda_2} = \infty \\ \text{This is } R = \text{minimum.} \end{array} \right. \end{aligned}$$

$$\begin{aligned} (2) = 0 \Rightarrow \frac{p_2}{A} &= e^{-Bx} [1 - p_2] \\ \text{Also, by definition of } A, & \\ \frac{p_2}{A} &= (1 - p_2) \frac{\sigma_1}{\sigma_2} \end{aligned} \left. \vphantom{\begin{aligned} (2) = 0 \Rightarrow \frac{p_2}{A} = e^{-Bx} [1 - p_2] \\ \text{Also, by definition of } A, \\ \frac{p_2}{A} = (1 - p_2) \frac{\sigma_1}{\sigma_2} \end{aligned}} \right\} \therefore e^{-Bx} = \frac{\sigma_1}{\sigma_2}.$$

The value of x obtained from this expression results in a maximum value of R . Replacing B in this expression by its definition in terms of σ_1 , σ_2 , and λ_2 , we obtain

$$\left(\frac{x}{\sigma_2} \right)_{\max} = \frac{\ln \left(\frac{\sigma_2}{\sigma_1} \right)}{1 - \frac{\sigma_1}{\sigma_2}}. \quad (A-2)$$

Equation (A-2) is plotted in Fig. 2 of the text. Note: Depth, $\frac{x}{\lambda_2}$, for which $R = \text{maximum}$, is independent of p_2 .

C. Value of R at $\left(\frac{x}{\lambda_2}\right)_{\max}$

Substitution of Eq. (A-2) into Eq. (A-1) and manipulation of results gives

$$R \text{ for } \left(\frac{x}{\lambda_2}\right)_{\max} \equiv R_{\text{peak}} = \left[1 + p_2 \left(\frac{\sigma_2}{\sigma_1} - 1 \right) \right] \left(\frac{\sigma_2}{\sigma_1} \right)^{-p_2}. \quad (\text{A-3})$$

Eq. (A-3) is plotted in Fig. 2.

D. Value of p_2 that Maximizes R_{peak}

$$\underbrace{\frac{dR_{\text{peak}}}{dp_2}}_{(1)} = \underbrace{\left(\frac{\sigma_2}{\sigma_1} \right)^{-p_2} \left\{ \left(\frac{\sigma_2}{\sigma_1} - 1 \right) + \left[1 + p_2 \left(\frac{\sigma_2}{\sigma_1} - 1 \right) \right] \ln \left(\frac{\sigma_2}{\sigma_1} \right) \right\}}_{(2)} = 0.$$

(1) $\neq 0$ for any $0 \leq p_2 \leq 1$, since $\sigma_2 \geq \sigma_1$ by definition.

$$(2) = 0 \implies (p_2)_{\max} = \frac{1}{\ln \left(\frac{\sigma_2}{\sigma_1} \right)} - \frac{1}{\frac{\sigma_2}{\sigma_1} - 1} \quad (\text{A-4})$$

Eq. (A-4) is plotted in Fig. 2.

E. Maximum Value of R_{peak}

Substituting Eq. (A-4) into Eq. (A-3) results in

$$(R_{\text{peak}})_{\max} = \left[1 + \left(\frac{\frac{\sigma_2}{\sigma_1}}{\ln \left(\frac{\sigma_2}{\sigma_1} \right)} - 1 \right) \right] \left(\frac{\sigma_2}{\sigma_1} \right)^{- \left[\frac{1}{\ln \left(\frac{\sigma_2}{\sigma_1} \right)} - \frac{1}{\frac{\sigma_2}{\sigma_1} - 1} \right]}. \quad (\text{A-5})$$

Eq. (A-5) is plotted in Fig. 2.

APPENDIX B

ENERGY WIDTHS OF TART CROSS-SECTION GROUPS

Figures B-1a, b, c, d, e, f, g, and h show the cross-section groups of the TART Monte Carlo code superimposed on the ^{235}U fission and total cross sections as plotted in Ref. 4.

Figures B-2a, b, c, d, e, and f make the same comparison for the ^{239}Pu cross sections.

Note that the TART cross-section groups are large, compared to the width of the ^{235}U and ^{239}Pu resonances at neutron energies below a few kilovolts.

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

(a)

(b)

(c)

(d)

(e)

(f)

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