

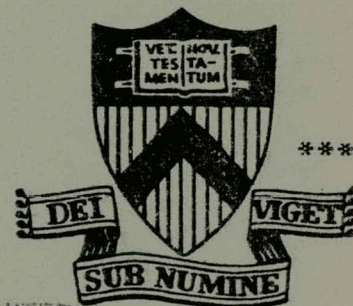
NEUTRONIC CALCULATION AND CROSS
SECTION SENSITIVITY ANALYSIS
OF THE LIVERMORE MIRROR FUSION/
FISSION HYBRID REACTOR BLANKET

BY

LONG-POE KU AND W. G. PRICE, JR.

**PLASMA PHYSICS
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ABSTRACT

The neutronic calculation for the Livermore mirror fusion/fission hybrid reactor blanket was performed using the PPPL cross section library. Significant differences were found in the tritium breeding and plutonium production in comparison to the results of the LLL calculation. The cross section sensitivity study for tritium breeding indicates that the response is sensitive to the cross section of ^{238}U in the neighborhood of 14 MeV and 1 MeV. The response is also sensitive to the cross sections of iron in the vicinity of 14 MeV near the first wall. Neutron transport in the resonance region is not important in this reactor model.

I. INTRODUCTION

The first part of this report describes a comparative study of fusion neutronic methods applied to the conceptual design of the Livermore fusion/fission hybrid reactor blanket.^(1,2) Neutron transport calculations were performed using a PPPL cross section library which was generated from ENDF/B-III. The results were compared with those reported by LLL based on the Livermore Evaluated Nuclear Data Library. By making a comparison we hope to discover any trend of discrepancy between the PPPL and LLL results. Our study shows that significant differences may appear. For instance the tritium breeding ratio, according to our calculation, would be lower by as much as 35%. Haight and Lee⁽³⁾ have shown that calculations using ENDF/B-III would in general give lower values for almost all the design parameters, including the tritium breeding, plutonium production and energy multiplication, the discrepancy in energy multiplication being the largest. Our results are different in that; (1) the largest difference found is for the tritium breeding and (2) the calculation using ENDF/B-III does not always underestimate the design parameters. For example, the plutonium production in our calculation was higher by ~15% compared to the Livermore calculation.

Because of the large differences observed, we have further investigated the effect of variation in neutron cross sections on the response calculated. This constitutes the second part of this report. We try to identify those portions

of the neutron life history for which the uncertainty in cross section has the greatest impact. Using the same blanket model, we found the tritium breeding capability of this reactor to be most sensitive to the ^{238}U cross section. In general, the tritium breeding is very sensitive to the high energy portion of the cross section.

In the following discussion, we describe the model of our calculation first (Section II). Section III presents the calculational results of some design parameters. Section IV gives the cross section sensitivity analysis. The conclusion is found in Section V.

II. MODEL FOR THE CALCULATIONS

For calculational convenience, most of the geometrical complexities were ignored. The reactor was modelled as concentric spherical shells, comprising the plasma region, the vacuum vessel, the fast fission zone, the tritium breeding blanket and the coil shield. Further, each spherical shell was assumed to contain a homogeneous mixture of materials. As a consequence of this simplification, the problem is suitable for one-dimensional calculation. A schematic description of the problem is illustrated in Figure 1. The nuclide densities used in the calculation are given in Table 1.

The D-T fusion neutrons were assumed to be born isotropically and uniformly in the central region of the reactor with an energy of 14 MeV. Two different plasma radii,

8.75 m and 2.40 m, were used in preliminary calculations. The differences in results due to the difference in plasma region size were found to be relatively small (e.g., 2% in the tritium breeding). For illustrative purpose, the plasma radius of 8.75 m is used in the following discussion.

In order to reduce the factors which could contribute to discrepancies in the result, we hoped to set up the model that resembles as closely as possible the one used in the Livermore calculation. Unfortunately, no single Livermore report could be found which gave a complete description of the data used to arrive at their results. Though most of the data given in Table 1 were taken directly from several Livermore reports,^(2,3) the uncertainty about some data makes the comparison less than definite. (In particular, the material composition of the coil shield was not available; we assumed it was stainless steel with the same composition as the vacuum vessel.)

III. TRANSPORT CALCULATION AND COMPARISON OF RESULTS

Both discrete ordinates and the Monte Carlo methods were used in the transport calculations; the computer code employed being ANISN⁽⁴⁾ and MORSE⁽⁵⁾ respectively. Both codes solve the Boltzmann equation in a multigroup fashion. A total of 30 groups were used. The group structure is given in Table 2. The same 30-group, P_3 neutron cross section data set was used for all PPPL analyses.

A comparison of the integrated neutron fluxes is shown in Figure 2. The fluxes are plotted as a function of distance from the first wall. The magnitudes of the fluxes at the first wall have been normalized using a wall loading of 1.15 MW/m^2 .

Clearly, the choice of stainless steel as the coil shield is not justified, since the flux of our calculation in this zone decreases much more slowly than that of the Livermore calculation. The fluxes in the fission zone and in the tritium breeding zone, however, should not be significantly effected by the incorrect representation of this region.

A comparison of some design parameters is shown in Table 3. These include the tritium breeding, plutonium production, energy multiplication, ^{238}U fission and ^{235}U fission. In general, the results of Monte Carlo calculation agree well with those of the ANISN calculation, considering the small number of histories used. Yet surprisingly large differences are observed between the Livermore results and ours. Compared to the Livermore results, our calculation underestimates the tritium breeding by as much as 30-40%, and overestimates the plutonium production by ~15%. However, the deviation in energy multiplication is only of the order of 2%.

Since the input specifications in our calculation were not all exactly the same as those used in the Livermore calculation, a certain degree of difference in results would be expected. On the other hand, it is unlikely that differences of the size observed are simply due to the differences in the input specifications. Another source of discrepancies could be

the difference in transport codes used. The LLL results were obtained with TART, a Monte Carlo code, while most PPPL calculations are made with ANISN, based on discrete ordinate methods. However, the basic simplicity of the model and the agreement of the ANISN and MORSE results suggests that this is not why the results differ.

We believe the differences more likely arise as a result of the differences in the basic neutron interaction data used. The Livermore calculation was based on data in the ENDL library. We have assumed that a published 175-group cross section set derived from ENDL⁽⁶⁾ adequately describes this data. The PPPL data set was obtained by collapsing the 100-group cross section set DLC-2F, using a hybrid blanket spectrum as the weighting function. In turn, DLC-2F was derived from ENDF/III. Self-shielding factors were applied for ^{238}U .

To illustrate the difference in cross sections, Figure 3 shows plots of the total and absorption cross section for ^{238}U . It is seen that in the resolved resonance region and in the 14 MeV vicinity the probability of absorption in the PPPL set is higher than that in the ENDL library. This is probably one of the reasons which accounts for the higher production rate for Pu and the lower breeding ratio for tritium obtained in our calculation.

Haight and Lee⁽³⁾ have made a study similar to this one. Significant differences were observed there also. They attributed the differences in results primarily to differences in the 14 MeV neutron-induced emission spectra. Our results

deviate from theirs in that calculations based on ENDF/B-III do not always give a lower value; and that the largest discrepancy is in tritium breeding rather than energy production.

To better understand the effect of variations of cross section on the neutron transport, we present some sensitivity analysis in the next section.

IV. CROSS SECTION SENSITIVITY STUDY

We use first order perturbation theory to study cross section sensitivity. We follow the method developed by Obloz et al.⁽⁷⁾. The only quantity examined here is the sensitivity of tritium breeding to various material cross sections. The forward and adjoint angular fluxes of the neutrons were computed by the ANISN code using P_3 - S_8 discretization. These fluxes were used subsequently as input to the code SWANLAKE⁽⁸⁾ to compute the sensitivity profile $(\Delta R/R)/(\Delta \Sigma/\Sigma_x)/\Delta U$. Here R is the total response of a given kind; Σ_x is the cross section of type x , which may represent the total, elastic, (n,α) or any other partial cross section data set; ΔU is the lethargy width of the energy group. The sensitivity function computed by SWANLAKE is thus the percentage change in total response due to one percent change in cross section of type x for a given energy group. The total response, R , considered here is just the tritium breeding ratio which can be computed by

$$R = \sum_{i=1}^I \sum_{g=1}^G \Sigma_{g,i} \phi_{g,i} V_i$$

where $\Sigma_{g,i}$ is (n,α) cross section for ${}^6\text{Li}$

$\phi_{g,i}$ is forward group flux

V_i is the interval volume

g is the group index, $g=1,\dots,G$

i is the spatial interval index, $i=1,\dots,I$

Alternatively, R can be computed by the adjoint fluxes

$$R = \sum_{i=1}^I \sum_{g=1}^G S_{g,i} \phi_{g,i}^* V_i$$

where $S_{g,i}$ is the source for the forward calculation

$\phi_{g,i}^*$ is the adjoint group flux.

In this particular case:

$$S_{1,1} = 1/V_1, \quad S_{g,i} = 0 \quad \text{if } g \neq 1, \quad i \neq 1$$

so that

$$R = \phi_{1,1}^*$$

R is 0.74253 or 0.74445 as computed by the forward or adjoint theory respectively.

IV.1. SENSITIVITY OF TRITIUM BREEDING TO THE CROSS SECTION OF ^{238}U

The sensitivity profiles of tritium breeding to the total cross section, (n,γ) reaction cross section and (n,f) cross section are given in Figures 4, 5 and 6. The sensitivity of tritium breeding to the fission χ is illustrated in Figure 7. Note that in SWANLAKE terminology, sensitivity to the "total" cross section really means sensitivity to the simultaneous variation of all cross sections by the same factor. (In these plots, the solid lines represent the negative values, and the dotted lines represent the positive values.)

Some major points of interest are discussed below:

(a) The sensitivity of tritium breeding to the total cross section of ^{238}U is positive at energies ≥ 5 MeV; and is negative ≤ 5 MeV, indicating that the tritium breeding is more sensitive to the "collision gain" at energies greater than 5 MeV and to the "collision loss" below 5 MeV. The positive sensitivity at high energy region is mainly due to the sensitivity to the fission cross section. The negative sensitivity is primarily due to the sensitivity to the (n,γ) reaction cross section.

(b) The tritium breeding is very sensitive to the total cross section at high energies. Two regions of particular interest are 1) the top group ($13.5 \text{ MeV} \leq E \leq 14.92 \text{ MeV}$), 2) the groups

with $100 \text{ keV} \leq E \leq 1 \text{ MeV}$. For the blanket model studied, 70% of the positive sensitivity to the ^{238}U total cross section is due to cross section for $E > 13 \text{ MeV}$, while 80% of the negative sensitivity is due to cross sections for energies between 100 keV and 1 MeV. This result is not surprising in view of the slowing down mechanisms of the neutrons contributing to the tritium breeding. The neutrons in the fission zone cannot be slowed down too quickly or too slowly. If they were slowed down too quickly without much spatial transport the chances of being absorbed by ^{238}U or other structural materials would be large, resulting in a loss. On the other hand, if they were slowed down too slowly, the multiple scattering processes at high energies would lead the neutrons to a premature leakage out of the system; since the $^6\text{Li}(n,\alpha)$ reaction cross section does not become appreciable until the neutron energies fall below 100 keV. Thus the neutrons contributing to the tritium breeding are most likely to be those which collide with ^{238}U nuclides at the early stage of their life history. Such collisions most likely result in the fission event, the $(n,2n)$ reaction or the (n,n') scattering to the continuum. Consequently the neutrons are transferred to the 1 MeV vicinity. Many collisions will then take place. The neutrons cross the fission zone boundary into the tritium breeding zone where further slowing down takes place. Eventually neutrons are absorbed by ^6Li . In fact, the average energy of the neutron flux at the fission-breeding borderline is $\sim 100 \text{ keV}$ (see Figure 8). It is quite clear, on the basis of above discussion, that the most sensitive region would be in the 14 MeV vicinity and in the 1 MeV neighborhood.

(c) The sensitivity to cross sections variations for neutrons with energy < 1 keV accounts for less than 1% of the total. Since a relatively small fraction of the neutrons contributing to tritium breeding are below 1 keV in the fission zone the ${}^6\text{Li}(n,\alpha)$ reaction is not sensitive to the cross section in this energy region at all. The detailed representation of resonances and interference minima thus does not seem to be of any particular importance. The result justifies the use of a few groups in the resonance region in the transport calculations.

(d) The sensitivity profile of tritium breeding to the (n,γ) cross section of ${}^{238}\text{U}$ indicates that the most sensitive region is between 20 keV and 1 MeV. The sensitivity in this energy region accounts for ~90% of the total (0.5125). It may be noticed that the tritium breeding is more sensitive to the (n,γ) reaction cross section than to the total cross section below 20 keV due to the increased contribution of (n,γ) reaction probability to the total collision probability. However, the sensitivity below 20 keV is only about 2% of the total, or $\Delta R/R = 0.01 (\Delta \Sigma / \Sigma)_{(n,\gamma)}$. The variation in (n,γ) cross section would result in the variation of tritium breeding of at most a few percent in this resonance region.

(e) The sensitivity profile of tritium breeding to the fission cross section of ${}^{238}\text{U}$ indicates that 54% of the sensitivity is due to the cross section in the top group, and 36% is due to the cross section in 1.5 - 6 MeV region. The sensitivity in

the energy region of 2 - 3 MeV alone accounts for ~15% of the total. The ${}^6\text{Li}(n,\alpha)$ reaction is not sensitive to the fission cross section in the energy region 6 - 10 MeV, even though the cross section rises to about 1 barn. This result is expected because fission and other reactions with source-energy neutrons predominantly transfer secondary neutrons below these energies. On the other hand the fission cross section falls off rapidly below 2 MeV. Since the tritium breeding is quite sensitive to the fission cross section in this neighborhood, the correct selection of group boundaries and the adequate representation of the cross section near the "peak" and "cliff" appear to be quite important.

(f) The shape of the sensitivity profile of the $\text{Li}(n,\alpha)$ reaction to the distribution of fission χ is similar to that of the χ -distribution itself, except the sensitivity profile drops more rapidly than the χ -distribution below 2 MeV. Again, the most sensitive region is in the 2 - 6 MeV region.

(g) The above discussions repeatedly emphasize the importance of the 1 - 6 MeV region. However, neutrons can reach this region only via nonelastic scattering to the continuum or by fission, the results thus suggest the importance of a correct representation of the secondary neutron emission spectra.

IV.2. SENSITIVITY OF TRITIUM BREEDING TO THE CROSS SECTION OF OTHER BLANKET MATERIALS

The sensitivity of tritium breeding to the total cross section of Fe, C, and O were also examined. The total sensitivities, i.e., the sensitivities summed over all spatial zones and energy groups, are shown in Table 4. It is clear from this table that among other blanket materials the tritium breeding is most sensitive to the cross section of iron. A plot of the sensitivity profile of tritium breeding to the total cross section of iron is given in Figure 9. We notice that there is a strong peak at the energy of the top group. The sensitivity in this group accounts for ~50% of the total. A study of the spatial dependence of the sensitivity function further reveals that about 50% of the sensitivity in the top group is contributed by the sensitivity in the region of the very thin first wall. In the 14 MeV vicinity the nonelastic collision probability is very high; the (n,2n) reaction alone accounts for about 1/3 of the total collision probability for each interaction. It has been reported that transport calculations for 14 MeV neutrons in iron using ENDF/B-III data grossly underestimate the fluxes in the several MeV region due to the incorrect representation of secondary neutron energy emission spectra. The calculation of neutron transport using ENDF/B-III data for the reactor model studied here would be expected to predict less ^{238}U (n,f) events. The discrepancies observed in Section III might be partly attributable to

discrepancies in the iron cross section near 14 MeV. However, the ${}^6\text{Li}(n,\alpha)$ sensitivity is probably mitigated by uranium fission, and there is good agreement between LLL and PPPL on the total amount of fission.

Another striking feature of Figure 9 is the relatively large negative sensitivity in the energy group of 0.5 - 1.25 keV. A more detailed examination of the spatial dependence of the sensitivity function shows that almost the entire sensitivity in this energy bin is contributed by the sensitivity in the tritium breeding region. This is of course not unexpected, since the flux spectrum in the tritium breeding region is considerably softer than that in the fast fission zone, yet the cross section of iron exhibits a very strong absorption resonance at 1 keV. In the energy region of 20 keV - 500 keV, where the cross section of iron exhibits more complicated resonance structure, the sensitivity accounts for ~40% of the total; and the majority of this is contributed by the sensitivity in the fast fission zone. The absolute magnitude of the sensitivity function in the resonance region, however, is small.

The vacuum vessel is actually made of stainless steel, which consists of Fe, Ni and Cr. The total sensitivity of tritium breeding to the total cross section of Ni and Co may reasonably be expected to be similar to that of the iron cross section, multiplied by the corresponding ratio of nuclear density (29% and 12% respectively).

The sensitivity of tritium breeding to the total cross sections of C, and O are considerably smaller, and will not be

discussed here. Other materials, such as Al, Mo, and ^{235}U , have relatively small concentrations. The sensitivity of tritium breeding to the cross sections of these materials will also be small.

V. CONCLUSION

In the course of studying the neutronic performance of the Livermore conceptual hybrid reactor blanket, we found large differences in the tritium breeding and plutonium production in comparing PPPL results to those reported by Livermore. According to our calculation, the tritium breeding would be 30 - 40% lower, while the plutonium production would be ~15% higher. The most probable source of these discrepancies is the cross section data used in the calculation. The cross section sensitivity study reveals that the tritium breeding capability in this reactor blanket is sensitive to the cross section variation for ^{238}U in the 14 MeV vicinity and in the 100 keV to 2 MeV region. The tritium breeding is also sensitive to the cross section of iron in the 14 MeV neighborhood in the region near the first wall. The resonance region which plays a very prominent role in the neutron transport in a fission reactor, does not seem to be of any particular importance here. We must point out, however, that the sensitivity study is strictly problem dependent. The results presented here may not be applicable to situations where other response functions are of interest.

VI. ACKNOWLEDGMENTS

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Table 1. Atomic Density in the
Blanket Model (atom/barn-cm)

<u>Zone No.</u>	<u>Nuclide</u>	<u>Density (cm-barn)⁻¹</u>
2	Cr	1.7600 -02
	Ni	7.1390 -03
	Fe	6.0400 -02
3	Cr	1.5136 -03
	Ni	6.1395 -04
	Fe	5.1944 -03
	²³⁵ U	1.6529 -04
	²³⁸ U	2.2504 -02
	Mo	4.2319 -03
4	Cr	1.5136 -03
	Ni	6.1395 -04
	Fe	5.1944 -03
	C	3.5288 -02
	⁶ L	2.3300 -03
	Al	2.3300 -03
	O	4.6600 -03
5	Cr	1.7600 -02
	Ni	7.1390 -03
	Fe	6.0400 -02

Table 2. Energy Group Structure

<u>Group No.</u>	<u>Upper Energy (MeV)</u>
1	1.4918 +1
2	1.3499 +1
3	1.2214 +1
4	1.1052 +1
5	1.0000 +1
6	9.0484 +1
7	7.4082 +0
8	6.0653 +0
9	4.0657 +0
10	2.7253 +0
11	1.8268 +0
12	1.4957 +0
13	1.2246 +0
14	8.2085 -1
15	4.9787 -1
16	3.0197 -1
17	1.1109 -1
18	2.4788 -2
19	5.5308 -3
20	1.2341 -3
21	4.5400 -4
22	1.6702 -4
23	6.1447 -5
24	2.2603 -5
25	8.3153 -6
26	3.0590 -6
27	1.8554 -6
28	1.1254 -6
29	6.8256 -7
30	4.1400 -7

Table 3. Comparison of Reaction Rate
for the Blanket Model

	$^{238}\text{U}(n,\gamma)$	$^6\text{Li}(n,\alpha)$	M^3	$^{238}\text{U}(n,f)$	$^{235}\text{U}(n,f)$
ANISN ¹	2.05	0.74	10.3	0.508	0.117
MORSE ²	2.12 \pm 6%	0.67 \pm 10%	10.0 \pm 11%	0.486 \pm 7%	0.128 \pm 9%
LLL ⁵	1.85	1.14	10.1	n.a. ⁴	n.a.

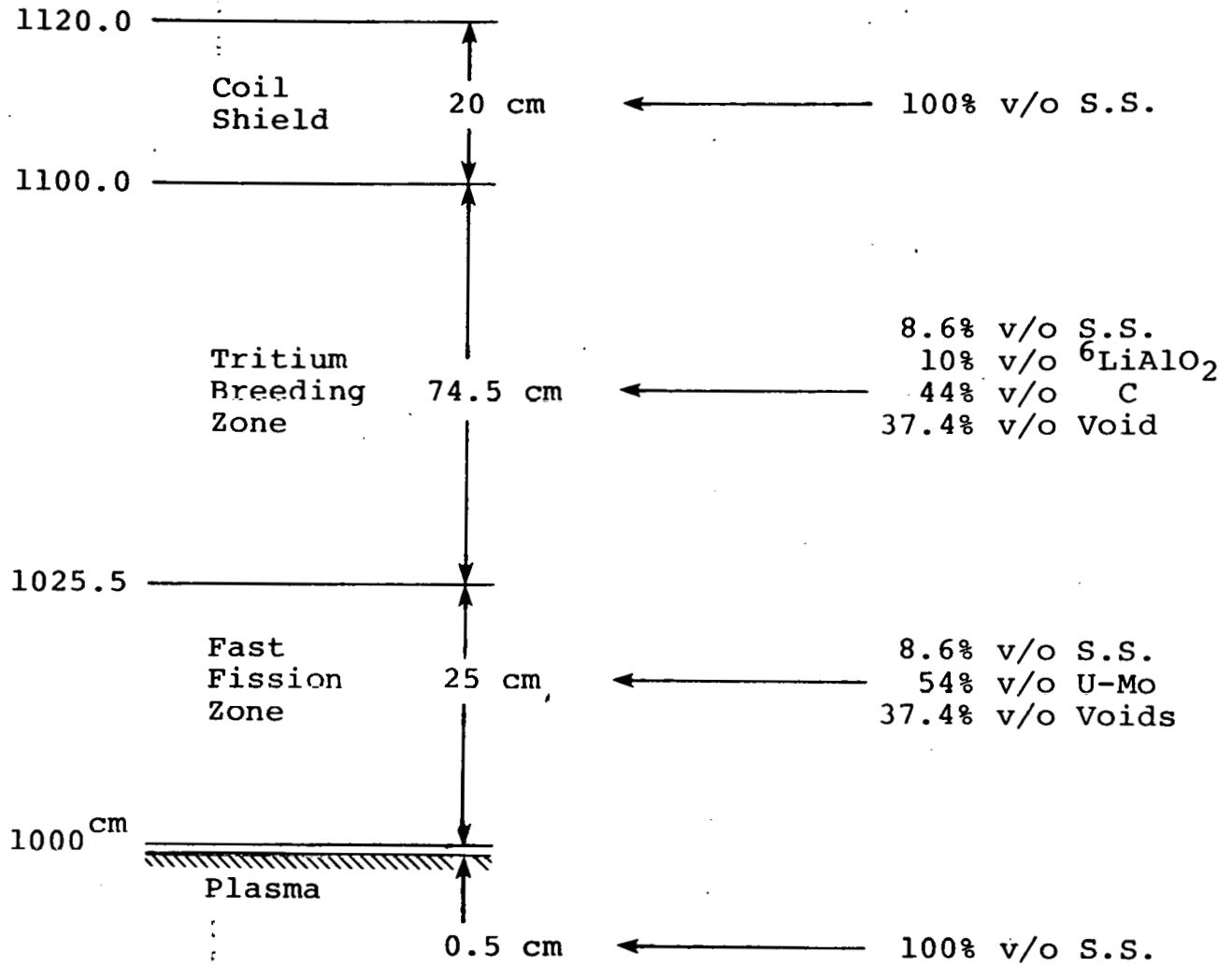
- Note: 1. ANISN P_3S_8 calculation
 2. MORSE 200 histories
 3. $M = (200 \text{ MeV} \times \text{total fission events} + 14 \text{ MeV}) / 14 \text{ MeV}$
 4. n.a.: not available
 5. from reference 2

Table 4. Sensitivity of Tritium Breeding to the
Total Cross Sections for Various Materials

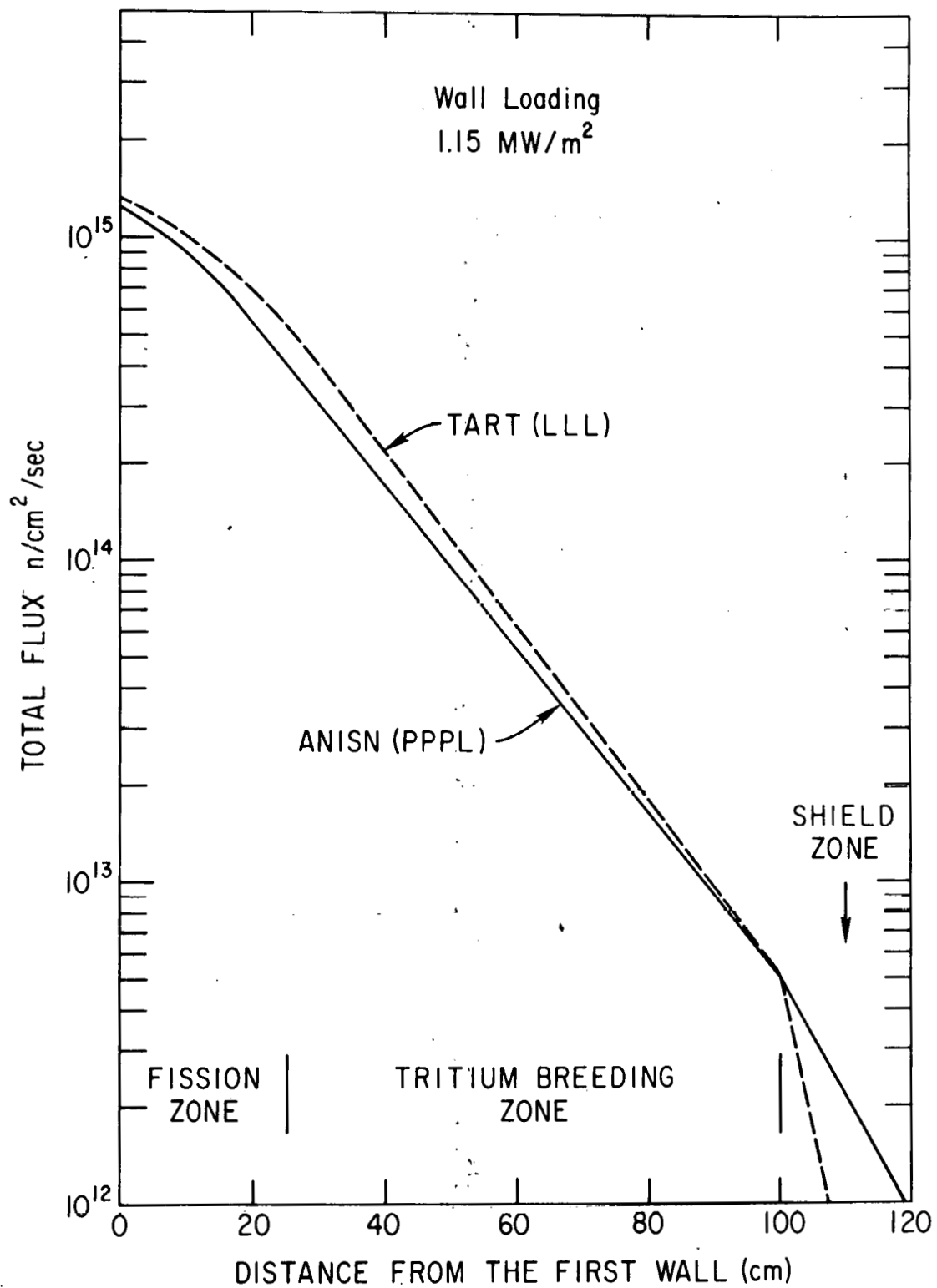
<u>Material</u>	<u>Integral Sensitivity*</u>
^{238}U	- 0.97293
Fe	- 0.19280
O	- 0.016907
C	- 0.076352

$$\text{Integral Sensitivity} = \int_{\mathbf{E}} \int_{\mathbf{r}} \left(\frac{\Delta R/R}{\Delta \Sigma_{\mathbf{x}}/\Sigma_{\mathbf{x}}} \right)_{\mathbf{E}, \mathbf{r}} d\mathbf{E} d\mathbf{r}$$

Figure 1. Geometric Model of the Livermore Reactor Blanket.

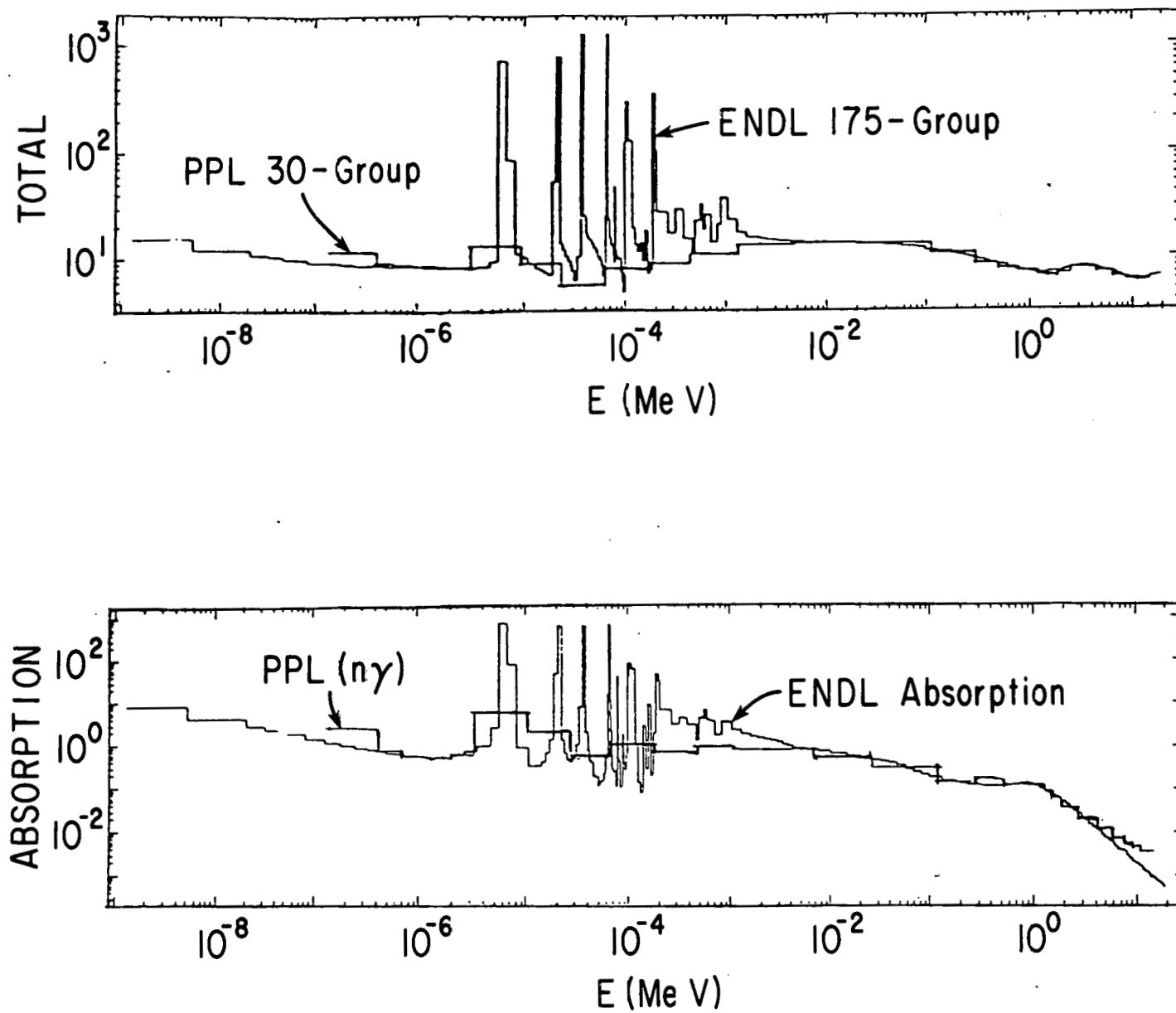


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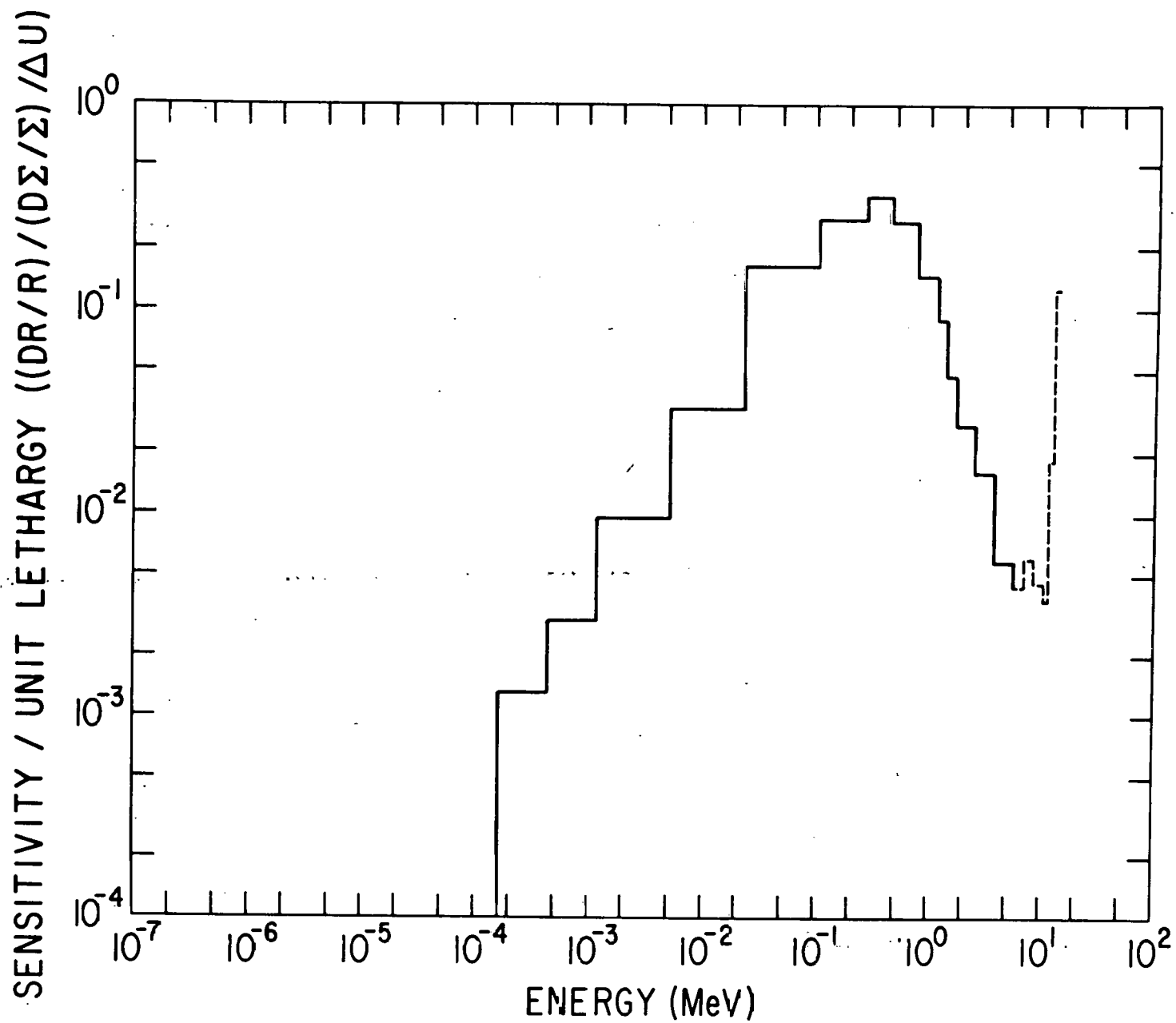
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Figure 2. Comparison of Integrated Neutron Fluxes.



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Figure 3. Total and Absorption Cross Section for ^{238}U .



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Figure 4. Sensitivity of Tritium Breeding to the Total Cross Section of ^{238}U .

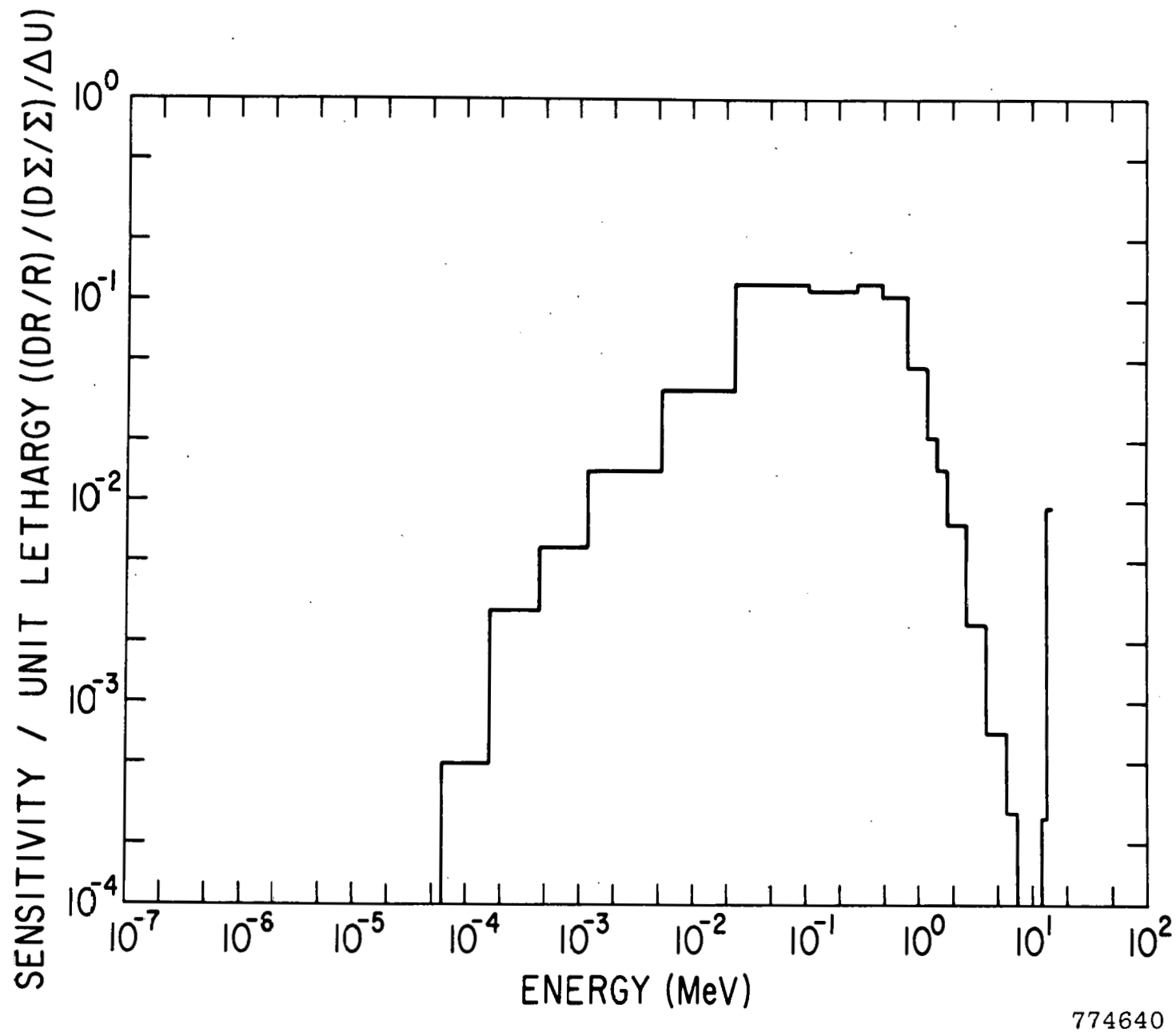
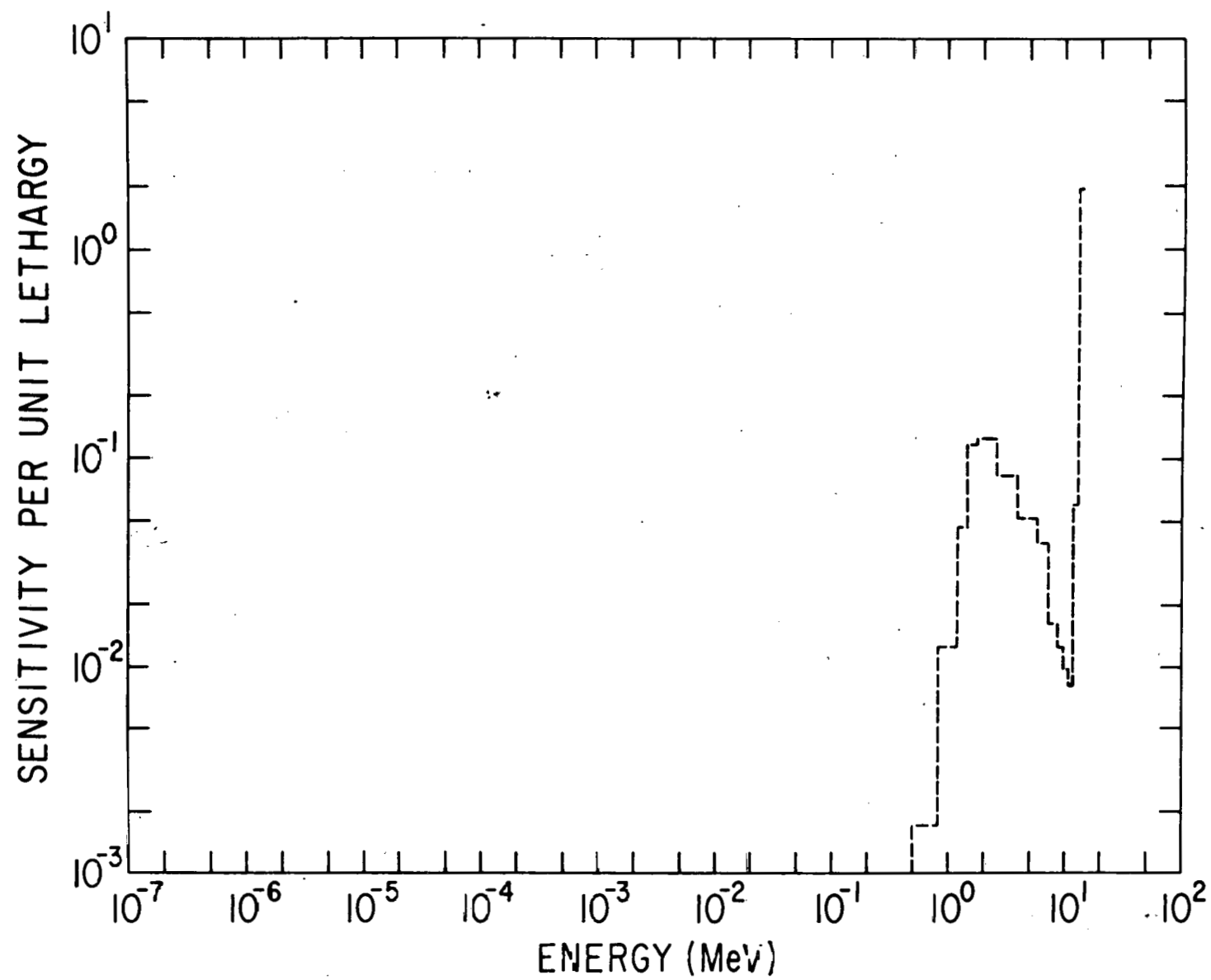
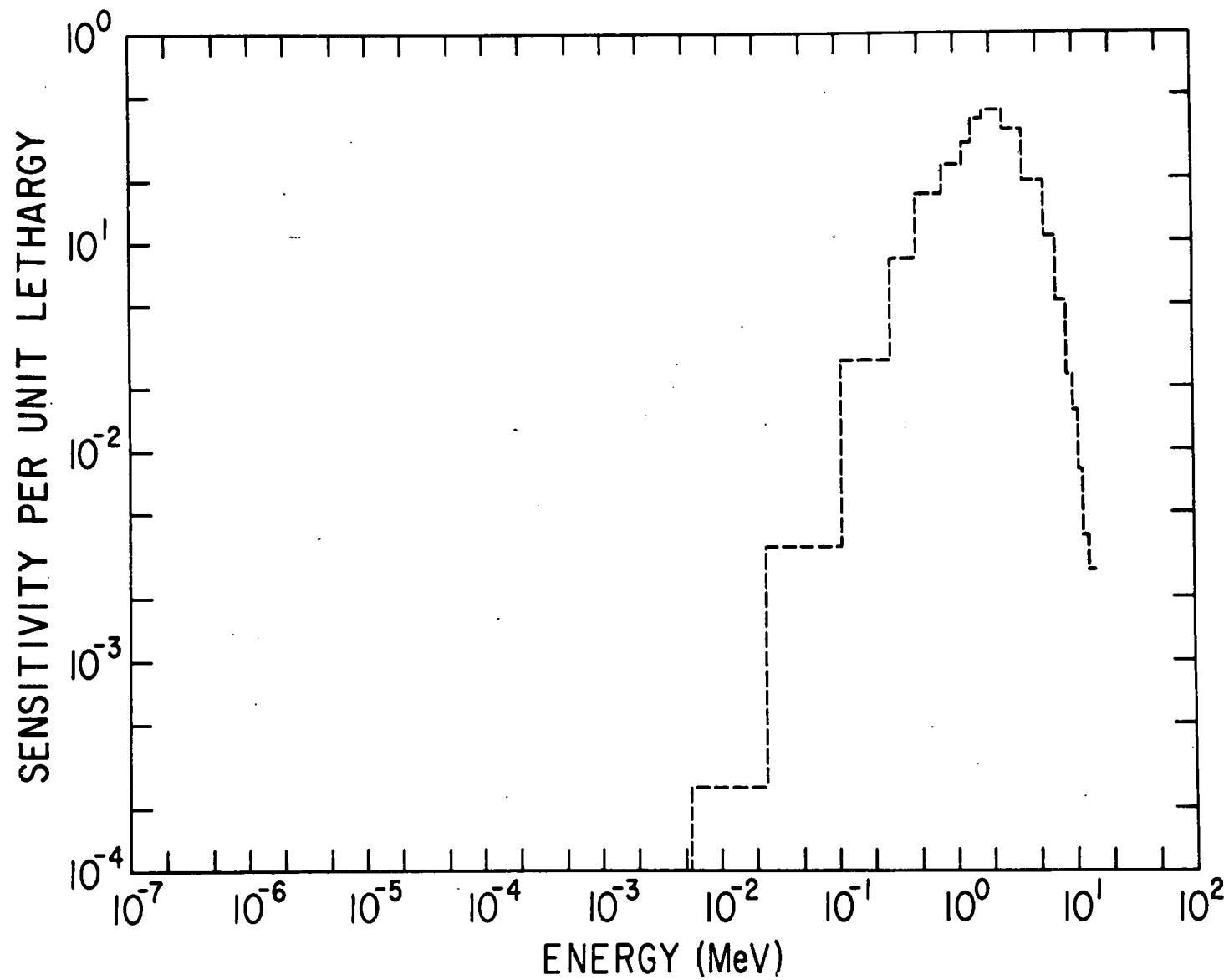


Figure 5. Sensitivity of Tritium Breeding to the (n,γ)
Cross Section of ^{238}U .



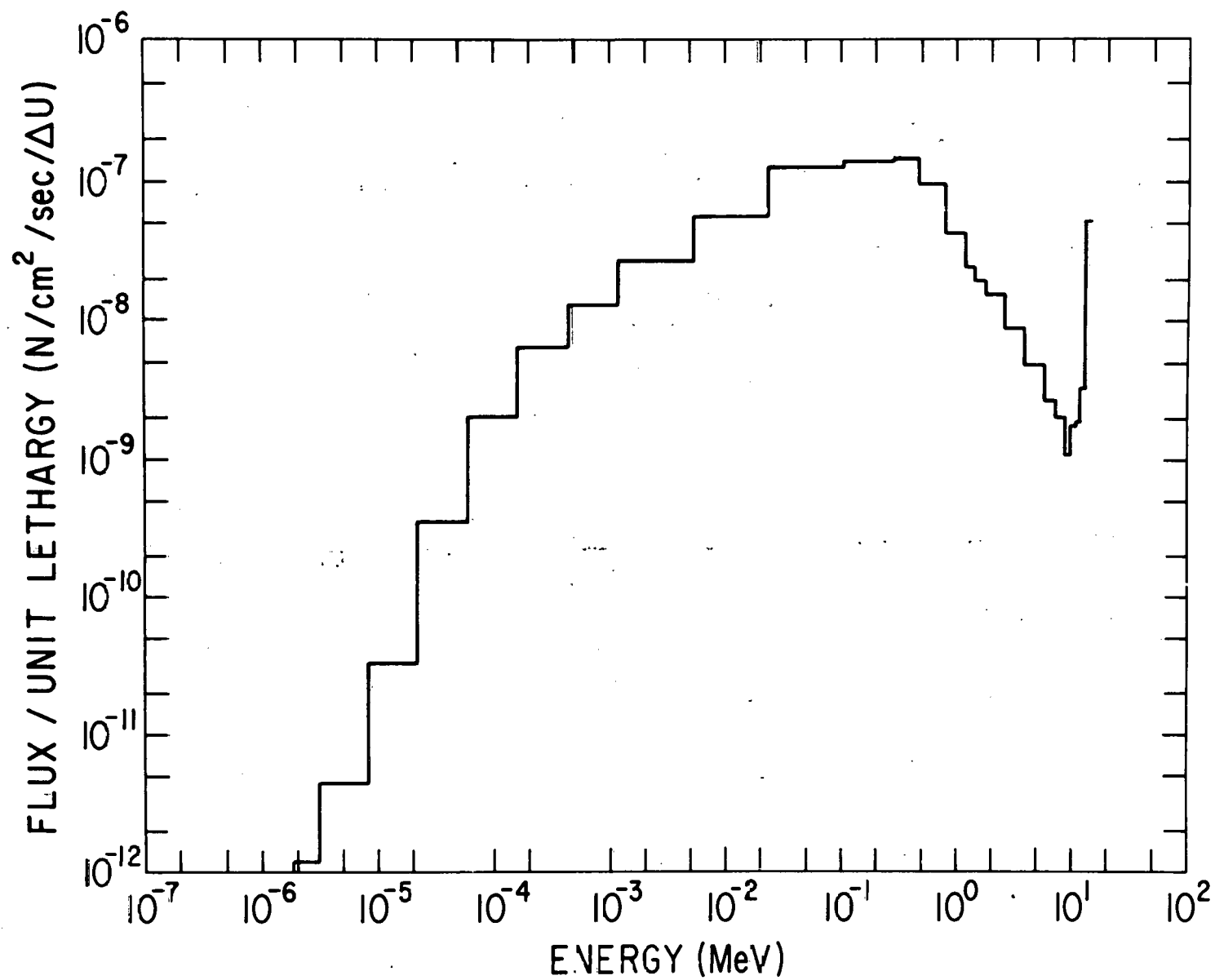
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Figure 6. Sensitivity of Tritium Breeding to the Fission Cross Section of ^{238}U .



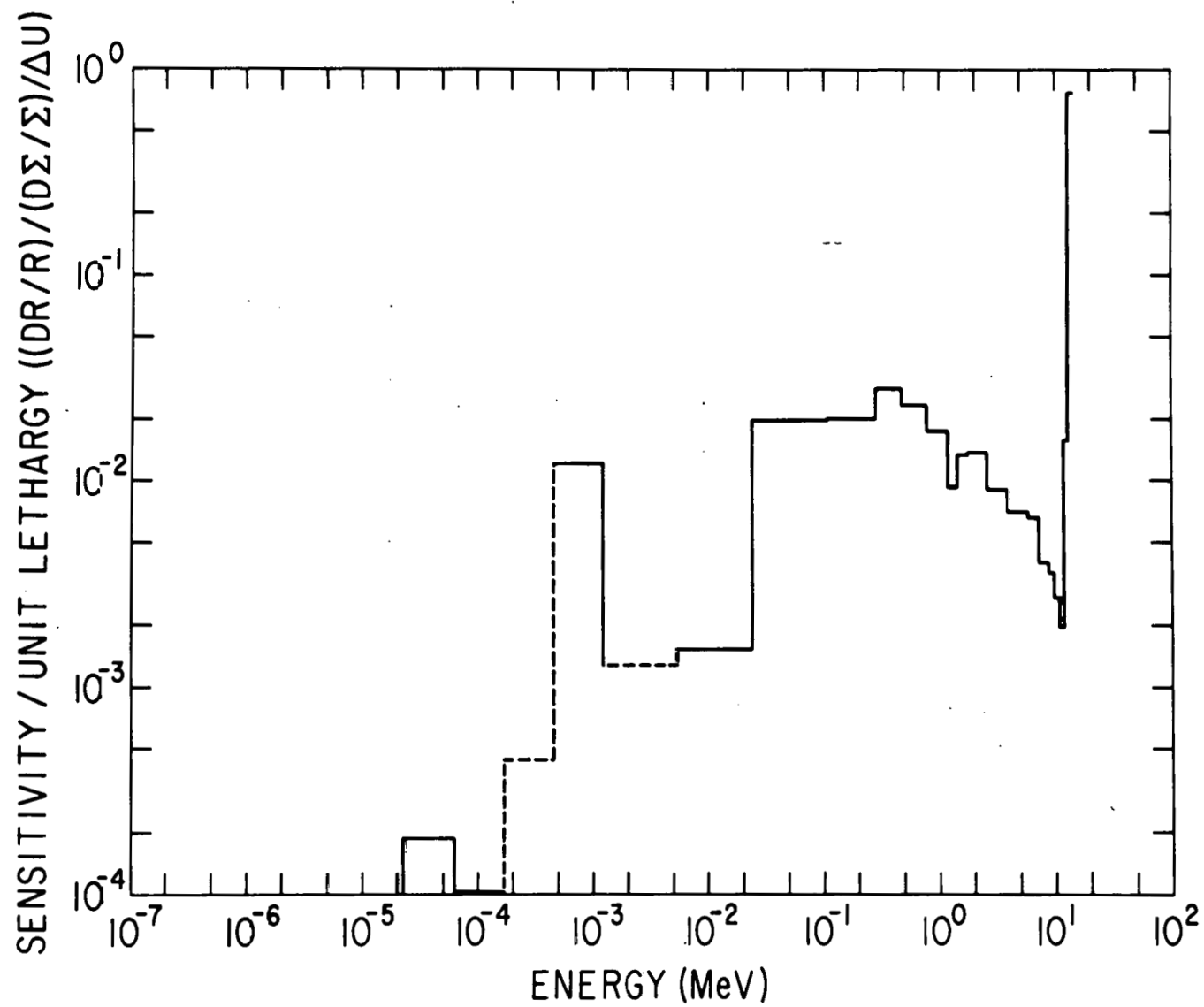
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Figure 7. Sensitivity of Tritium Breeding to ^{238}U Fission χ distribution.



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Figure 8. Flux Spectrum at the Interface between Fast Fission Zone and Tritium Breeding Zone.



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Figure 9. Sensitivity of Tritium Breeding to the Total Cross Section of Iron.