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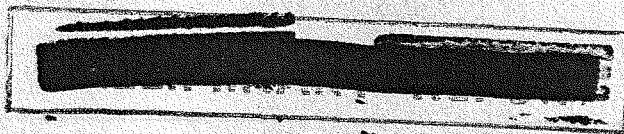
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Dragon Project Report



A COMPARISON OF CODES FOR  
SPECTRUM AND REACTIVITY CALCULATIONS

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by

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A COMPARISON OF CODES  
FOR SPECTRUM AND REACTIVITY  
CALCULATIONS

by

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ABSTRACT

A comparison of sets of codes for calculation of spectrum, broad group cross sections, and reactivity is described.

The comparison has shown the significance of the leakage term (the buckling) introduced into the spectrum code and the disadvantages of the group partition used when this comparison was performed.

A number of differences of the basic input cross sections have been found and their effects investigated.

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1. Fast Reflector Spectra from General Atomic Calculations

# A COMPARISON OF CODES FOR SPECTRUM AND REACTIVITY CALCULATIONS

by

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## 1. INTRODUCTION

The purpose of the calculations described in this report has been to compare the methods which are used by General Atomic and by the Dragon Project for the calculation of neutron spectrum and reactivity for a Dragon type reactor. By this comparison a number of deviations in the input data (cross sections) and the numerical procedures of the codes have been disclosed and effects, which hitherto have been underestimated, have been investigated.

This report discusses mainly the significant effects which have been found, while the codes are only described briefly.

## 2. CALCULATION METHODS

The codes used for the comparison by General Atomic are the following:

GAM - I: Spectra calculation and constants averaging in the fast energy range [1].

The main features are:

- (a) The  $P_1$  equations are integrated over quarter lethargy units from 10 MeV to 0.414 eV, yielding a total of 68 groups.
- (b) A fission source is used for calculating the spectrum.
- (c) The energy-angle correlation is retained for slowing down in all isotopes; i.e. a full scattering matrix is included for both the  $P_0$  and  $P_1$  scattering terms.
- (d) It is possible to introduce an energy dependent buckling.
- (e) Inelastic scattering and (n, 2n) processes are included.
- (f) Resonance absorption is treated according to the methods developed by F. T. Adler, G. W. Hinman and L. W. Nordheim [4].
- (g) Self-shielding factors can be included for any nuclide.
- (h) A predetermined spectrum may be used as input to the code.

GATHER I: Spectra calculation and constants averaging in the thermal energy range.

The main features are:

- (a) The programme covers the energy range below 2.1 eV in 96 groups.
- (b) A slowing down source is used for calculating the spectrum.
- (c) 96 point scattering kernels are included in the library for various scatterers. For graphite they are calculated with the gas model at high temperatures and with Parks model at low temperatures.
- (d) It is possible to introduce an energy dependent buckling.
- (e) Self-shielding factors can be included for every nuclide.
- (f) A predetermined spectrum may be used as input to the code.

GAMBLE: A two dimensional, multi-group diffusion theory code with up to ten groups and arbitrary scattering matrix. The programme was used first with the same six group structure as used by Dragon for Angie and later for ten group calculations with six thermal and four fast groups.

The codes, which have been used mainly for the Dragon calculations until recently, are:

STEWPO: Calculates spectrum in 43 groups and broad group average cross-sections for the just-critical-core and for a reflector [5].

ANGIE: A two dimensional multi-group diffusion theory code. The main difference from GAMBLE is that scattering is only allowed from each group to that immediately preceding and to the two following groups. Used in 6 group calculations in this comparison.

During the last part of the calculations performed the code MUPO was available.

MUPO: This code corresponds to Stewpot but the library cross-sections (except the graphite scattering cross-sections) are created from the General Atomic Library by a condensation to 43 groups. The code offers the possibility of performing spectrum calculations both for a bare critical reactor - as Stewpot, and for a given leakage - as GAM and GATHER [2].

Finally the effects of the variations of average group constants for 6 groups - as given by the General Atomic codes, Stewpot and Mupo have been investigated by simple calculations of the infinite multiplication factor  $K_{\infty}$  determined from these 6 group data (Mercury programme 5461).

### 3. CALCULATIONS - RESULTS AND DISCREPANCIES

The results for the effective multiplication factor  $K_{\text{eff}}$  as obtained by Angie and Gamble are given in Table 1. The reactor considered was the Dragon reactor with a two zone core. The inner zone has Th/U atomic ratio  $N = 20$ , while  $N = 0$  for the outer zone.

The first comparison obtained for the  $K_{\text{eff}}$  was between calculation Nos. 1 and 2 in the table, and as the difference  $\Delta K_{\text{eff}} = 0.031$  between the two results was rather disappointing, a somewhat larger investigation of the discrepancies was initiated.

Some of the main reasons for the differences are indicated in Table 1, while the discussion of the differences is given in the following list.

#### 3.1 Buckling Dependence

The neutron spectrum and the average group cross-sections calculated depend on the leakage term - the buckling  $B^2$  - which is used in the calculation. Stewpot iterates on the buckling until criticality is achieved and the values are for the hot case:

$$\text{Core 1: } B_1^2 = -7.6 \times 10^{-6} \text{ cm}^{-2} \approx 0$$

$$\text{Core 2: } B_2^2 = +14.1 \times 10^{-4} \text{ cm}^{-2}$$

Just fortuitously these figures are not very far from the best values if the energy independent buckling is to be used. In the General Atomic codes, Gam and Gather, the buckling is introduced as input data, and for the first series of calculations the bare core buckling:

$$B_1^2 = B_2^2 = 24.4 \times 10^{-4} \text{ cm}^{-2}$$

was used, partly because no better values were available and partly because calculations done on the General Atomic HTGR Critical Assembly core 7 had shown the insignificant effect of buckling. (This later appeared to be due to a better group structure and to the fact that the core composition was uniform and that the core radius was larger.)

The effects of a change  $\Delta B^2$  in buckling depend on the energy boundaries and the cross sections of the groups. For the 6 group partition used, group 5 is especially sensitive. This has been shown by Mupo for core 1 in Tables 2 and 3. (The groups are numbered as in Angie so that the slowest group is group No. 1.) Table 2 shows that a change  $+ \Delta B^2 = 24.4 \times 10^{-4} \text{ cm}^{-2}$  for core 1 gives for group 5:

$$\Delta \Sigma_{s,\text{out}} = -26\%$$

$$\Delta \Sigma_{\text{abs}} = -15\%$$

where  $\Sigma_{s,\text{out}}$  and  $\Sigma_{\text{abs}}$  respectively are the macroscopic cross sections for scattering out and absorption. From Table 4 calculation No. 3 it is seen that this decreases  $K_{\infty}$  for core 1 by  $\sim 3\%$ . The total effect for

Table 1  $K_{eff}$  for Dragon - Two Zone Core

Calculation No.	Temp.	Input Data	Diffusion Code	No. of Groups	$K_{eff}$	Deviation		Reasons for Deviation
						Calc.	%	
1	Hot	Stewpot	Angie	6	1.104			
2	"	GA = $G_{am} + G_{ather}$	Gamble	6	1.073	1-2	2.9	$B^2$ , $\nu$ , cross sections
3	"	"	"	10	1.107	2-3	3.0	Energy groups partition
4	"	"	Angie	6	1.082	2-4	0.7	$\nu$
5	"	Core = Stewpot Reflector = GA	"	6	1.107	1-5	0.3	Reflector data
6	"	GA*	Gamble	6	1.098	2-6	2.3	No upscattering above 1 eV
7	"	GA**	"	10	1.120	3-7	1.2	$B^2$
8	"	MUPO (Stewpot) (Buckling)	Angie $\Delta$	6	1.115			
9	"	MUPO (GA) (Buckling)	" $\Delta$	6	1.095	8-9	1.8	$B^2$
10	Cold	Stewpot	Angie	6	1.166			
11	"	GA	Gamble	10	1.179	10-11	1.1	Energy partition $B^2$ , $\nu$ , cross sections
12	"	GA**	"	10	1.185	11-12	0.5	$B^2$

GA\* - No upscattering above 1 eV

GA\*\* - Corrected bucklings

Angie  $\Delta$  - Not a full Rz geometry calculation - only calculation  
8 and 9 should be compared

Table 2 Cross Sections for Group No. 5 (second fastest group)

	Stewpot	MUPO	MUPO	GAM		
$B^2$	0	0	24.4	24.4	$m^{-2}$	
$\Sigma_{s,out}$	0.003737	0.003633	0.002883	0.002812	$cm^{-1}$	Scattering out
$\Sigma_{abs}$	0.001800	0.001957	0.001709	0.001632	$cm^{-1}$	Absorption

Table 3 Changes in MUPO Cross Section with the Buckling  $B^2$

$$\text{Changes in per cent: } \Delta\Sigma = \frac{\Sigma(B_1^2) - \Sigma(B_2^2)}{\Sigma(B_1^2)} \cdot 100\%$$

$$\text{Core 1. } B_1^2 = 24.4 \cdot 10^{-4} \text{ cm}^{-2}, B_2^2 = 0$$

$$\text{Core 2. } B_1^2 = 24.4 \cdot 10^{-4} \text{ cm}^{-2}, B_2^2 = 14.1 \cdot 10^{-4} \text{ cm}^{-2}$$

Group No.	Core 1		Core 2		$\Delta B_R^2 \cdot 10^{+4} \text{ cm}^{-2}$
	$\Delta\Sigma_{abs}$	$\Delta\Sigma_{s,out}$	$\Delta\Sigma_{abs}$	$\Delta\Sigma_{s,out}$	
Fast = 6	+ 0.3	- 2.4	- 0.2	- 0.88	10
5	- 14.5	- 26.4	- 6.5	- 10.1	1
4	- 3.4	- 7.8	+ 0.68	- 3.1	3
3	- 1.1	- 2.6	- 0.58	- 1.2	9
2	- 0.5	- 1.6	- 0.18	- 0.71	20
Slow = 1	- 0.03	- 0.0007	- 0.01	- 0.0007	$\approx$ 400

$\Delta B_R^2$  produces roughly a change  $\Delta\Sigma_{s,out} = 1\%$  }  
 or  $\Delta\Sigma_{abs} = 0.4\%$  } for both cores 1 and 2

all groups of  $\Delta B_1^2$  is seen from calculations 5 and 6, Table 4:  $\Delta K_\infty = 4.1\%$  for core 1. For core 2 the buckling effect appears to be smaller and from calculation No. 15 a  $\Delta K_\infty = 0.3\%$  is obtained. Calculations 8 and 9 of Table 1 show that the effect on  $K_{eff}$  of these buckling changes for cores 1 and 2 is 1.8%.

The effects of the buckling depends on the group boundaries and, as the group partition used has a large lethargy width for group No. 5 the effect is large. A better group energy partition will decrease the significance of the buckling. This fact is also quite clear from the 10 group calculations 3, 7, 11 and 12 in Table 1, where the changes in  $K_{eff}$  are smaller.

### 3.2 Energy Boundaries for the groups

The energy boundaries chosen for the 6 group calculations were as shown in Table 6. It has already been mentioned that this group structure makes the results far too dependent on the buckling.

Moreover, at high temperature there is a considerable amount of upscattering from group 3 to group 4, which includes some of the lower very significant resonances. Those upscattered neutrons will physically only enter into the region of group 4 below the resonances. In this group formulation, however, they are absorbed according to the average cross section for the group, including the contributions of the resonances. This results in too great an absorption of the upscattered neutrons and thus too low a multiplication factor is obtained. If the absorption of the neutrons scattered up is neglected, which corresponds to neglecting the scattering up from group 3 to 4, the effect on  $K_\infty$  is, for core 1,  $\Delta K_\infty = +3.8\%$  and for core 2,  $\Delta K_\infty = +1.5\%$ ; see Table 4. For  $K_{eff}$  the change is +2.3% according to Table 1 calculation No. 6.

For the Gamble - Angie comparison in Table 4, calculation 1-2, this effect of the group partition is, however, less important as they are practically identical. The above changes correspond to a 100% decrease of the cross-section for scattering up  $\Sigma_s 3 \rightarrow 4$ , while the actual difference between Stewpot and General Atomic data is 11% which means that the Stewpot  $\Sigma_s 3 \rightarrow 4$  will correspond to ~0.26% higher  $K_{eff}$  than the General Atomic  $\Sigma_s 3 \rightarrow 4$ .

### 3.3 Dependence on $\nu$

The number  $\nu$  of neutrons produced per fission depends on the energy of the neutrons producing the fission, but the effective value is for Stewpot 2.452, while, for General Atomic codes and for Mupo, it is 2.430. (The latter is considered to be the best available value.)

This difference goes directly into the value of  $K_{eff}$  and explains 0.9% of the deviation listed in Table 1, calculations 2 and 11. Furthermore, it explains the result of calculation 4, Table 1.

It must be noticed that this discrepancy does not enter Table 4, as  $\nu = 2.452$  is used for all calculations of  $K_\infty$ .

### 3.4 Dependence on the Scattering Down from Group 4

The cross section  $\Sigma_s 4 \rightarrow 3$  for the scattering down from the group No. 4 just above thermal energy (>1 eV) was in the original comparison practically the same for Gam and Stewpot. However, an anomaly was found [3] in the Stewpot spectrum owing to an error in the scattering data. This was corrected in Mupo and then the  $\Sigma_s 4 \rightarrow 3$  obtained by MUPO was ~18% higher than that obtained from Gam. The main reason for this discrepancy is presumably that the Gam data are calculated independently of Gather and the neutrons scattered up from the region below 1 eV are not taken into account. These neutrons would increase the spectrum in the lower part of group 4 and would give as a result a higher value of  $\Sigma_s 4 \rightarrow 3$ . The corresponding change in the absorption cross section is small.

It must be pointed out that the effect of neutrons scattered up is much less significant if a higher boundary energy e.g. ~2 eV were chosen between group 3 and 4. The energy partition used is thus very unsuited for the General Atomic codes.

The significance of the change is investigated in calculations Nos. 7 and 16 of Table 4, where  $\Delta K_\infty$  for cores 1 and 2 respectively is -3.1% and -1.3% when  $\Delta \Sigma_s 4 \rightarrow 3$  is ~-18%. The reason for this rather large change in  $K_\infty$  is that the neutrons are transferred down into a group where  $\eta$  is approximately increased by 1.

### 3.5 Dependence on the Scattering Model

The scattering model used in Stewpot and Mupo calculations is the Schofield crystal model at all temperatures. Input to the programmes is a scattering matrix obtained from a 60 point kernel integrated over a flat flux on the energy range 0.001  $\rightarrow$  0.1787 eV and from a 40 point kernel integrated over a  $\frac{1}{E}$  flux on the range 0.1787  $\rightarrow$  33.74 eV. Input to Gather is a 96 point kernel calculated with the Parks crystal model in the cold case, and the gas model in the hot (1300°K) case.

As a result, rather large discrepancies are found for the thermal scattering cross sections, but as shown in calculation 12, Table 4, for Core 2 the change in  $K_\infty$  is small for the hot case. This is explained by the fact that the changes of  $\eta$  are rather small in the thermal region.

### 3.6 Reflector Data

The group data for the reflector are in Stewpot calculated for a spectrum created by neutrons started at fission energies in an infinite medium.

At General Atomic the reflector data have been obtained in the following way:

In the fast energy range (GAM) the cross sections have been averaged over input spectra. These spectra have been obtained by a multigroup one dimensional (radial) calculation of the reactor. The reflector has been divided in two regions: the first inner

Table 4  $K_{\infty}$  Calculations

6 Group Data	Calculation No.	Core	$B^2 \cdot 10^4 \text{ cm}^{-2}$	$K_{\infty}$	Deviation		Remarks
					Calcu.	%	
Stewpot	1	1	0	0.9975			
GA	2	1	24.4	0.9421	1-2	5.6	
Stewpot	3	1	0	0.9685	1-3	2.9	GA data for group 5
GA	4	1	24.4	0.9776	2-4	3.8	No scattering up >1 eV
MUPO	5	1	24.4	0.9685	2-5	2.7	
MUPO	6	1	0	1.0094	5-6	4.1	
MUPO	7	1	24.4	0.9393	5-7	3.0	$\Sigma_{s,4 \rightarrow 3}$ decreased 19%
Stewpot	8	1	0	0.9811	1-8	1.7	MUPO data for group 5
Stewpot	9	2	14.1	1.8833			
GA	10	2	24.4	1.8519	9-10	1.6	
Stewpot	11	2	14.1	1.8828	9-11	0	GA data for group 5
Stewpot	12	2	14.1	1.8813	9-12	0.1	$\Sigma_{s,out}$ thermal from GA
GA	13	2	24.4	1.8792	10-13	1.5	No scattering up >1 eV
MUPO	14	2	24.4	1.8671	10-14	0.8	
MUPO	15	2	14.1	1.8724	14-15	0.3	
MUPO	16	2	24.4	1.8479	14-16	1.3	$\Sigma_{s,4 \rightarrow 3}$ decreased 18%

$\nu = 2.452$  has been used in these calculations

10 cm, and an outer region. The fast spectra for the 2 regions are plotted in Figure 1. In the thermal energy range the GATHER code has been run in the usual way (spectra calculated from a slowing down source).

These two procedures have given somewhat different results for the group cross sections, but the significance for  $K_{\text{eff}}$  is small - see Table 1, calculation 5. The effect on the power peak at the core-reflector boundary could be somewhat bigger.

### 3.7 Cross Sections

A large number of cross sections are read into the codes from their respective library tapes. The following list gives the main differences found so far:

- (a) Fast fission data are included in Gam and Mupo, but not in the Stewpot library.
- (b) Stewpot library tape No. 21 was used in the comparison and this is a rather old library tape with a very low thermal (= non resonance) cross section for thorium.
- (c) The thorium resonance data used in Mupo and Gam are the same - both corresponding to the resonance integral 84 b in infinite dilution, while the resonance integral for the Stewpot library tape No. 21 is 95 b. The difference in Table 2 for  $\Sigma_a$  given by Mupo and Gam for group 5 may be explained by the different methods of calculating the resonance cross sections, while the difference between Mupo and Stewpot is explained by the fact that the largest resonance is laying below 33 eV - in group 4, and this resonance is much higher in Stewpot than in Mupo. The contribution of this high resonance in group 4 for Stewpot is, however, cancelled by the effect of the U-235 data mentioned in d.
- (d) The General Atomic data used in Mupo give ~ 30% higher capture cross section for U-235 in group 4 and this leads to a decrease of  $K_{\infty}$  especially for core 2.
- (e) When the microscopic group averaged cross sections are compared for Mupo and Gam, large differences are found for U-238 in groups 4 and 5. This may be explained by the difference in calculation methods and the fact that the energy boundary between groups 4 and 5 is 33.74 eV in Mupo, while in Gam it is 37.27 eV, and a large U-238 resonance is in that interval. This cross section is, however, not very significant for  $K_{\infty}$  or  $K_{\text{eff}}$  as the amount of U-238 is small.
- (f) Large differences between transport cross sections for U-235 and U-238 have been found, but these are not significant, as the carbon is the isotope which determines the transport cross section.

The total effect of the input cross sections - with the energy partition used here - can be estimated from the Mupo/Stewpot calculations 1-6 and 9-15 in Table 4, when the effects of  $\Sigma_s 4 \rightarrow 3$  given in calculations 7 and 16 are taken into account. This leads in both core 1 and 2 to a change of  $\sim -1.9\%$  in  $K_{\infty}$ .

### 3.8 Resulting Differences in $K_{eff}$ and $K_{\infty}$

When the Mupo and the General Atomic six group constants are compared, it is seen that the  $K_{\infty}$  obtained is practically the same if the same buckling is used in the Mupo and the General Atomic calculations and the difference in  $\Sigma_s 4 \rightarrow 3$  is taken into consideration.

When Mupo and Stewpot are compared and it is taken into account that  $\nu$  in Mupo is lower than in Stewpot, it is seen that the resulting  $K_{\infty}$  is the same for core 1, while for core 2 Mupo gives  $\sim 1.5\%$  lower result. This difference is the result of two factors with opposite effects: generally the General Atomic data used for Mupo gives a lower  $K_{\infty}$ , but the corrected value of  $\Sigma_s 4 \rightarrow 3$  gives a higher  $K_{\infty}$ . For core 1 the two effects just accidentally cancel one another.

The total effect on  $K_{eff}$  of the factors mentioned are summarised in Table 5. When the rather large uncertainty of the single figures is taken into account, it is seen that the original disappointing difference between calculations 1 and 2, Table 1 is explained.

The change of  $K_{eff}$  from the earlier calculation (calculation 1, Table 1) to the calculations including all improvements and using Mupo or Gam + Gather is estimated in Table 5, and this shows that a small increase of  $K_{eff}$  is to be expected. This is also demonstrated by calculation 7, Table 1, which is supposed to be the most rigorous performed so far.

## 4. CONCLUSION

The comparison has shown the significance of the buckling introduced in the spectrum calculation, and future spectrum calculations must include a buckling which has been determined from earlier calculations. The procedure will in that case be the following: to start with a guess on the bucklings and to calculate with it the constants for a first diffusion calculation, out of which the proper bucklings can be determined. This will normally lead to energy dependent bucklings. Several methods for the buckling calculations are possible but it must be mentioned that the buckling is space dependent and thus a suitable average buckling must be used.

Furthermore, the comparison has shown the disadvantages of the energy group partition used here. A new partition must, according to the results, avoid groups of large lethargy width, as these are especially buckling dependent. The upper limit of the highest thermal group must be high enough not to have upscattering above it, otherwise the upscattered neutrons will go in a group with a cross section artificially too high. A good boundary for this kind of high temperature reactor appears to be equal to or above 2 eV.

The General Atomic data used in the General Atomic codes and Mupo are

Table 5 Changes in  $K_{eff}$  in per cent

Reason for Change	Change in $K_{eff}$ Calculation 1-2 Table 1	Change in $K_{eff}$ From Calculation 1 to future
Cross section	~ - 1.9	~ - 1.9
$\nu$	- 0.9	- 0.9
Buckling $B^2$	- 1.8	~ 0
Scattering $\Sigma_s, 4 \rightarrow 3$	~ + 0.7	~ + 2
$\Sigma_s 3 \rightarrow 4$ and Energy partition	~ + 0.26	~ + 2.3
Total	- 3.6	+ 1.5
Change "experienced"	- 2.9	+ 1.5*

\*Comparison of calculations 1 and 7, Table 1

Table 6 Six Group Energy Partition

Group	Energy
1	0.001 - 0.0225 eV
2	0.0225 - 0.3568 eV
3	0.3568 - 1 eV
4	1 - 33.74 eV
5	33.74eV - 0.8208 MeV
6	0.8208 - 10 MeV

Table 7

10 Group Energy Partition:  
Energy Boundaries from Highest down

$10^7$   
 $0.67379 \times 10^5 \text{ eV}$   
 $0.1013 \times 10^3$   
 $0.1371 \times 10^2$   
 $0.19 \times 10^1$   
0.40  
0.20  
0.10  
 $0.40 \times 10^{-1}$   
 $0.15 \times 10^{-1}$   
 $0.50 \times 10^{-2}$

found to be more pessimistic than the Stewpot data, but they are recommended for future use as they are of a later date.

The large difference between the calculations originally intended for comparison has been explained. The changes and corrections proposed here have rather a large effect - up to ~2% each on the reactivity but, as some of them cancel each other, the total effect on the reactivity of the Dragon reactor is expected to be a small positive change.

The comparison has not shown any difference between the multi-group diffusion codes Angie and Gamble when the same input data are used.

5. ACKNOWLEDGMENT

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"Stewpot" A 43 Group Code for Calculation of Neutron Spectra and Multigroup Constants  
D.P. Report 60

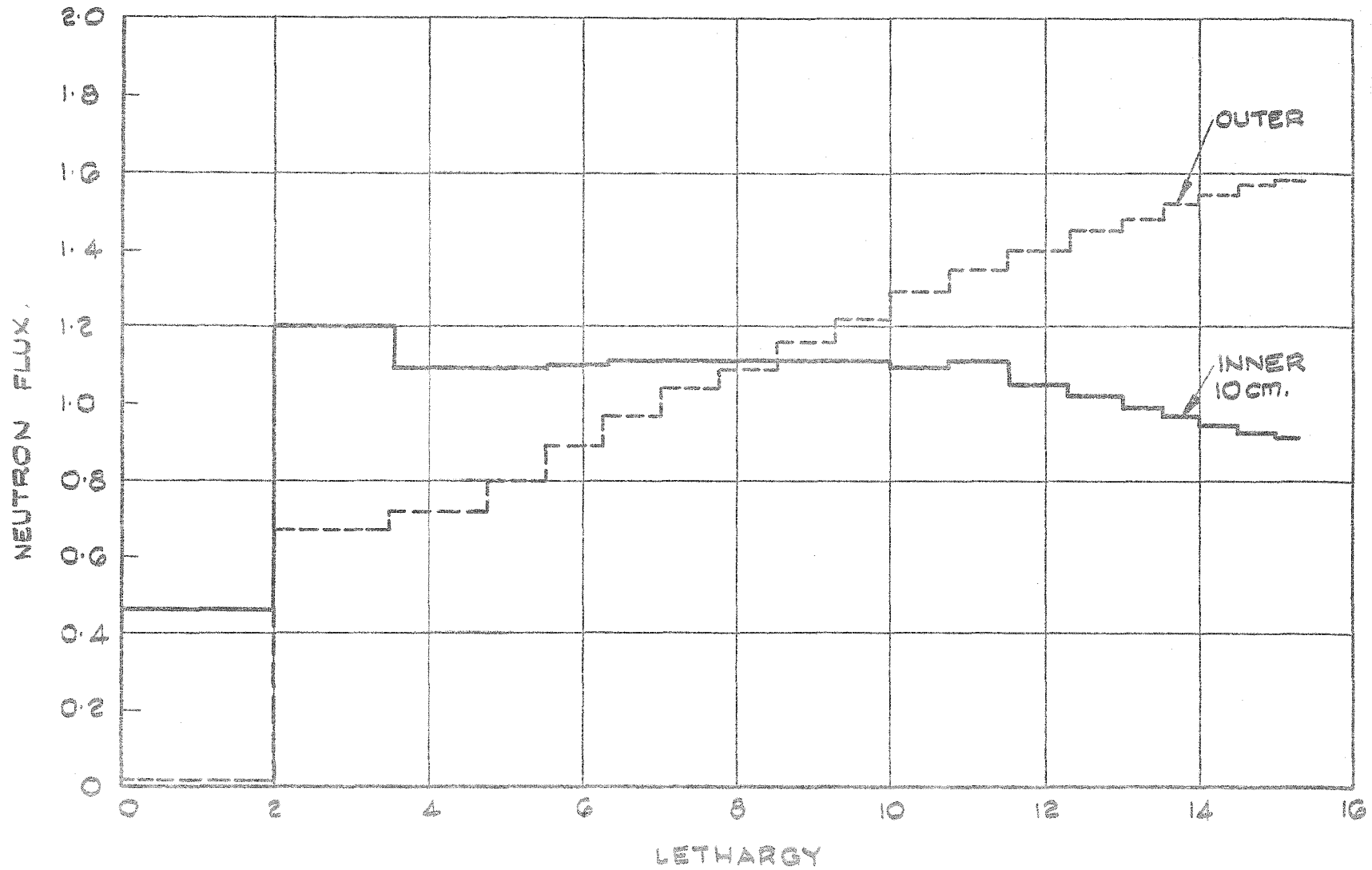


FIG.1 FAST REFLECTOR SPECTRA FROM GENERAL ATOMIC CALCULATIONS.