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Updating of the Leopard Data Library

L. Henrique Claro, Artur da Cunha Menezes Filho

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UPDATING OF THE LEOPARD DATA LIBRARY

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ABSTRACT

The LEOPARD library is being updated and tested for typical PWR unit cells with enrichments ranging from 1.0 to 4.1%(W/o) and H_2O:U ratios varying from 1.0 to 10.0.

A reasonably good agreement with experimental values for some spectral indices is obtained if the fission cross-section of ^{235}U is reduced by 0.6% in the thermal range and by 20% in the epithermal range, the epithermal capture cross-section for ^{235}U is increased by about 20% and the number of neutrons per fission in the thermal range of ^{235}U is increased by 0.8%.

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I. INTRODUCTION

Although the LEOPARD code [1] was developed in the late 1950s, it is still widely used for calculations of typical cells of thermal reactors.

Even though it contains various approximations, the code is extremely useful when applied to light-water-moderated reactors because the input data are easy to prepare and little computing time is required and, in particular, because it has a burn-up calculation option.

In its most widespread version the LEOPARD code uses a library of cross-sections based on data from the B-II version of the Evaluated Nuclear Data File (ENDF/B-II). In order to reproduce the multiplication factor (K_{ef}) for critical cells typical of thermal reactors some adjustments have been made in the library, mainly in the number of neutrons per fission. It is interesting to note, however, that adjustments taking K_{ef} as an integral reference parameter may mask errors which cancel out. In that case the adjustment effort made for a cell at the beginning of the reactor lifetime may be lost in the course of burn-up because other isotopes have come to form part of the system.

In its original version the LEOPARD library contains 9 elements with resonance information, not including certain structural materials such as iron, nickel, etc., and 16 elements with inelastic scattering information, plutonium-240, -241 and -242 not being considered explicitly.

The purpose of the work discussed here is to produce a LEOPARD library based on the ENDF/B-IV data, which may not be the last word in basic data, but which do represent a reasonably great advance beyond ENDF/B-II, especially as regards resonance information.

The IEAv's version of ENDF/B-IV does not contain lumped fission product data. Since the work on establishing this file is still in progress at IEAv, all the lumped fission product cross-sections of the new library will be the same as in the older library.

Section II of this paper presents all stages of the preparation of a decimal intermediate library (SPOTD file) for subsequent conversion to binary form by the SPOTS program. It also indicates the modifications made in the SPOTS program to give it access to the new library. As a result of the modifications in SPOTS the user must also make some changes in the LEOPARD code. These are described in Section III. Section IV gives a detailed description of certain cells used as reference cells. The adjustments and results are presented in tables and diagrams in Section V, and Section VI offers some conclusions.

II. PREPARATION OF THE LIBRARY

The preparation of a new library for the LEOPARD code calls for the use of various processing codes. Since the calculation models used in the thermal energy range (E < 0.625 eV) are different from the procedures applied in the epithermal range (E > 0.625 eV), different codes are required for these two energy ranges. In general, the ETOG code [2] is used for epithermal energies and the ETOT code [3] for the thermal range of the spectrum.

The combined processing of ENDF/B-IV by the chain ETOG + ETOT for each of the 25 elements in the LEOPARD library leads to a decimal file called SPOTD which is used as input for the SPOTS program, which in turn generates the binary library for the LEOPARD code. This processing chain is represented in Fig. II.1.

II.1. Generation of data for the thermal range (0-0.625 eV)

For the thermal energy range the ETOT code with the TEMPEST option was used in 172 energy groups. The weighting factor used for this range was of the 1/E type, as various tests with other weighting spectra had shown a complete insensitivity of the cross-sections with respect to the choice of spectrum.

In IEAv's version the ETOT code has no access to file 7 of ENDF/B-IV (low-energy scattering law). Since it was necessary to calculate the cross-sections for hydrogen and deuterium, those isotopes being bound in the molecules H_2O and D_2O, respectively, the FLANGE-2 code [4] was used for this purpose.

II.2. Generation of data for the epithermal range (0.625 eV-10 MeV)

In the epithermal energy range the ETOG code with the MUFT option was used in 54 energy groups. The weighting function used was of the type 1/E + fission spectrum.

In the LEOPARD code, (n,2n) reactions are treated as fission reactions with a number of neutrons per fission equal to 2. The use of this option in the ETOG code implies that the elements nickel, zirconium, chromium, deuterium and samarium have "fission" cross-sections different from zero. Calculations performed for instrumentation cells and fuel poison cells typical of PWR-type reactors, where physically fissile isotopes are absent, lead to absurd results, because LEOPARD tries to calculate the buckling value for criticality in a system where this operation is devoid of meaning.

The solution adopted was to add the "fission" cross-sections for those five elements to the inelastic scattering cross-sections (one of the options of the ETOG code). Various tests were carried out and yielded negligible differences in the important integral parameters between one approach and another.

II.3. Generation of a binary library for the LEOPARD code

In the old version of the SPOTD file the thermal library was prepared in 246 energy groups for subsequent condensing to the 172 groups actually used by LEOPARD. This condensing was done by the SPOTS program by means of interpolation. In its new version the thermal file of SPOTD is generated in 172 energy groups, which makes it possible to omit the COFE subroutine and the TERP function from the SPOTS program. This approach is clearly superior to the original one, as it avoids interpolation errors and reduces the computing time for SPOTD→SPOTS→library processing.

In addition to these modifications the reading system of the SPOTS program was altered to improve the utilization of memory capacity.

The original version of the LEOPARD library contained nine elements with resonance information and 16 elements with inelastic scattering matrix information. Processing with the ETOG code indicated, for the new library, the existence of 17 elements with resonances and 22 elements with an inelastic scattering matrix. In order for these modifications to be accessible to the SPOTS program the dimensions of the variables NRIG, LRIG, EM, R, ALPHA, PROB and SI had to be redefined in accordance with Table 1.

III. MODIFICATIONS IN THE LEOPARD CODE

In order to make the LEOPARD code consistent with the new structure of the SPOTS program the modifications indicated in Table 1 must also be carried out in the LEOPARD code.

To calculate the resonance escape probability the LEOPARD code uses, as a first approximation, the values derived from the resonance integral calculated by means of an empirical correlation [5]. The scattering cross-section values to be used must be equal to those of the potential cross-section. In the original version, these values were the same as those in group 45 of the elastic scattering cross-section. In the new version, the elastic scattering cross-section for ^{238}U in group 45 of the epithermal range is different from the potential cross-section, hence it is necessary to introduce some modifications so as to ensure

that the calculation by way of the empirical correlation is not altered. The user must therefore make the following changes in the MUFT subroutine:

Old version	Updated version
EQUIVALENCE (EN,VFAST (1)),(SS,SSC(1,45))	EQUIVALENCE (EN,VFAST (1))

Elimination of the equivalence between SS and SSC implies that the variable SS, read in INPUT, is transmitted to the MUFT subroutine through a COMMON of the COMMON/IEAV83/SS(25) type, which must be present in the INPUT, THRMAL, INGR and MUFT subroutines and in the QD function. In order to avoid compilation errors the variable SS (which was defined in SPOTS, but was not used by LEOPARD) must be replaced by some "silent" variable.

Table 2 shows, in condensed form, the modifications which the user must introduce in order to make the updated library accessible to the LEOPARD code.

IV. DESCRIPTION OF STANDARD PROBLEMS OF LIBRARY ADJUSTMENT

In tackling the adjustment of the new LEOPARD library a total of 35 problems [5,9-11] were selected to simulate typical unit cells of pressurized light-water reactors with enrichments between 1.0 and 4.1% (W/o) and H_2O:U ratios between 1.0 and 10.0.

Table 3 presents the physical characteristics of ten of these standard problems.

V. ADJUSTMENTS AND RESULTS

V.1. Adjustments

In analysing the results produced by the new library by means of the LEOPARD code the following spectral indices were used as reference parameters for adjustment purposes:

ρ^{28}: Ratio of epithermal capture rate to thermal capture rate for ^{238}U;

δ^{25}: Ratio of epithermal fission rate to thermal fission rate for ^{235}U;

δ^{28}: Ratio of total fission rate for ^{238}U to total fission rate for ^{235}U;

C^{*}: Ratio of total capture rate for ^{238}U to total fission rate for ^{235}U; and

K_{ef}: effective multiplication factor.

The procedures used previously [5,6] to adjust the LEOPARD library took as a reference value the multiplication factor for typical cells of PWRs. The expectation was that a good prediction of K_{ef} would mean small errors in the reaction rates. In fact, it is possible, as a result of errors cancelling out, for reaction rates with reasonably large deviations from the measured values to produce fairly accurate multiplication factor values. In the work discussed here, therefore, the multiplication factor has been adjusted after the spectral indices, these having proved to be relatively insensitive to variations in the number of neutrons per fission.

Analysis of the results produced by the new library (without ajustment) indicated a tendency towards underestimating ρ^{28}, δ^{28} and C^* and overestimating δ^{25}. On the basis of this observation, and using a heuristic procedure, the combination of adjustments which best eliminates those tendencies was found to be:

(1) To reduce by 0.6% the values of the thermal fission cross-sections for ^{235}U;

(2) To reduce by 20% the values of the epithermal fission cross-sections for ^{235}U;

(3) To increase by 20% the values of the epithermal capture cross-sections for ^{238}U; and

(4) To increase by 0.8% the value of the number of neutrons per fission (thermal range of ^{235}U).

V.2. Results

Tables 4-8 compare results from the original library with results from the adjusted library for the standard problems described in Section IV. It may be seen that in about 85% of cases the new library predicts the spectral indices with a smaller divergence from the measured values than the old library does.

V.3. Comparison of results for a typical cell of the Angra I reactor

As was already pointed out above, the LEOPARD code is much used for calculations involving fuel burn-up. In the absence of experimental values, the performance of the updated library has been verified in terms of the results produced by the original library for certain selected integral parameters.

The input data used in LEOPARD for the cell are represented in Table 9. Results on the ^{240}Pu production rate, ^{235}U consumption rate, conversion rate (ratio between capture in fertile isotopes and absorption in fissile isotopes) and infinite multiplication factor are represented, for 10 degrees of burn-up (burn-up $\leq$ 14 000 MW·d/t) in Figs 1-4.

Figures 5 and 6 show microscopic thermal absorption cross-sections for ^{240}Pu and microscopic thermal capture cross-sections for ^{239}Pu, indicating that the old library (ENDF/B-II) tended to underestimate these values as compared with the updated library (ENDF/B-IV).

VI. CONCLUSIONS

It must be stressed that the adjustment of a library is directly related to the type of problem to which the library is to be applied. For this reason, there is no standard adjustment for different groups of users. Codes like LEOPARD, which generate cross-sections for other codes (e.g. CITATION [8]), must, in keeping their libraries adjusted, take as reference not the value of the multiplication factor but the value of the reaction rates and/or spectral indices.

The most correct procedure for adjusting the LEOPARD library is to minimize the differences between calculated and measured values throughout one burn-up cycle. In general, these experimental values are not available at the LEOPARD stage, but only at a later stage, e.g. after processing by codes such as CITATION.

In our work we have tried to reduce the differences between calculated and measured values while staying within the various limitations imposed by the existing approximations in the code. For example, some of the cells analysed have a very small pitch, which invalidates the use of an equilibrium spectrum in the thermal range (Wigner-Wilkins) to condense the cross-sections. Besides, the narrow resonance model (NR approximation) used to calculate the flux in the epithermal range leads to error when applied to the broad resonances which exist at low energies.

Thus, for the range of enrichments and H_2O:U ratios studied we can conclude that the new library based on ENDF/B-IV calculates with reasonably good precision the parameters of typical unit cells of light-water reactors. It should be noted that the adjustment was performed for cells with fresh fuel, i.e. cells in which no fission products or isotopes formed by radiative capture were present. The practical verification of

the quality of the nuclear data on the plutonium and/or fission product chain can be carried out on the basis of the user's experience.

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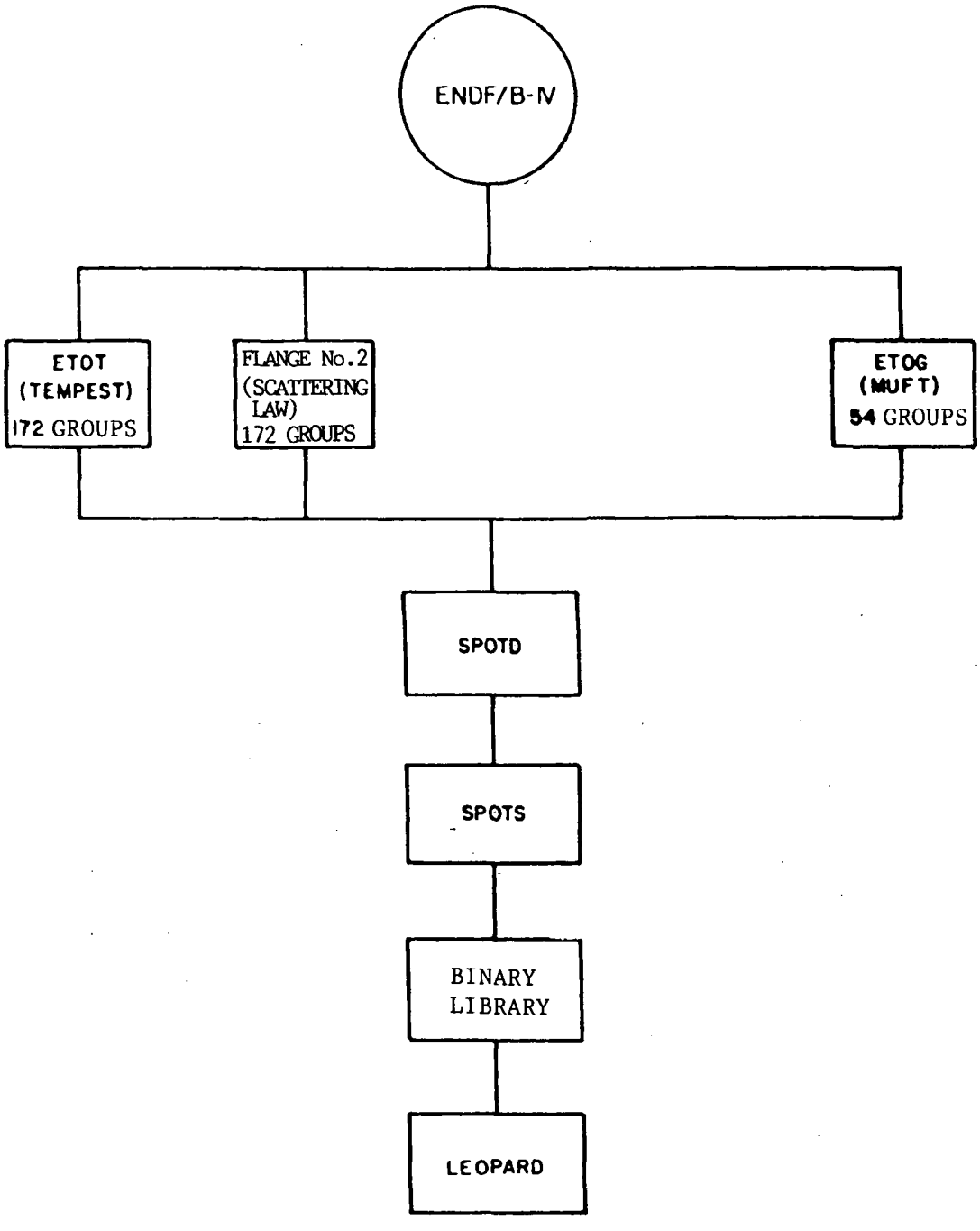

Fig. II.1: Flow diagram for the preparation of the LEOPARD library.

OLD VERSION	UPDATED VERSION
NRIG(10,30)	NRIG(17,30)
LRIG(10,30)	LRIG(17,30)
EM (200)	EM (700)
R (200)	R (700)
ALPHA(200)	ALPHA(700)
PROB(325,16)	PROB(325,22)
SI (16,54)	SI (22,54)

Table 1: Modifications in the SPOTS program.

ORIGINAL VERSION	UPDATED VERSION	SUBROUTINE OR FUNCTION TO BE MODIFIED
PROB(325,16)	PROB(325,22)	
NRIG(10,30)	NRIG(17,30)	MUFT, SLOW
LRIG(10,30)	LRIG(17,30)	RESINT, ED34
EM(200)	EM(700)	
R(200)	R(700)	
ALPHA(200)	ALPHA(700)	
EQUIVALENCE (EN,VFAST(1)),(SS, SSC(1,45))	EQUIVALENCE (EN, VFAST(1))	MUFT
SS(25)	WW(25)*	INPUT, THRMAL, INGR, MUFT, QD
NONE	COMMON/IEAV83/SS(25)	INPUT, THRMAL, INGR, MUFT, QD

Table 2: Modification in the LEOPARD code.

(*) "silent" variable

CASE	COMPOUND	ENRICHMENT (W/o)	H_2O : U	DENSITY (g/cm^3)	PELLET DIAMETER (cm)	CLADDING MATERIAL	OUTER DIA. OF CLADD. (cm)	THICKNESS OF CLADD. (cm)	PITCH (cm)	B^2 (m^2)	MOLAR FRACTION D_2O	$N(B^{10})$: N(U235)
TRX-1	U-METAL	1,3	2,35	(b)	0,983	AL	1,1506	0,0711	1,8060 (c)	57,00	0,	0,
TRX-2	U-METAL	1,3	4,02	(b)	0,983	AL	1,1506	0,0711	2,1740 (c)	54,69	0,	0,
BAPL-1	UO_2	1,328	2,88	10,53	0,9728	AL	1,1506	0,0711	1,5580 (c)	32,59	0,	0,
BAPL-2	UO_2	1,328	3,58	10,53	0,9728	AL	1,1506	0,0711	1,6520 (c)	35,47	0,	0,
BAPL-3	UO_2	1,328	4,83	10,53	0,9728	AL	1,1506	0,0711	1,8060 (c)	34,22	0,	0,
YCE-1 (a)	UO_2	2,734	2,18	10,18	0,7620	SS-304	0,8594	0,04085	1,0287 (d)	40,75	0,	0,
WAP-1 (a)	UO_2	2,734	10,38	10,18	0,7620	SS-304	0,8594	0,04085	1,6891 (a)	52,92	0,	0,
BAW-1 (a)	UO_2	3,745	4,51	10,37	0,7544	SS-304	0,8600	0,0406	1,2522 (d)	38,39	0,	0.0374
BAW-2 (a)	UO_2	4,069	2,55	9,46	1,1278	SS-304	1,2090	0,0406	1,5113 (a)	44,00	0.4966	0
BAW-3 (a)	UO_2	4,069	2,55	9,46	1,1278	SS-304	1,2090	0,0406	1,5113 (a)	14,23	0,6970	0,0062

Table 3: Description of some standard problems used in adjusting the LEOPARD-code library.

(a) Used only to adjust the multiplication factor;

(b) For metallic uranium cells it is more convenient to give the concentrations instead of the volume (^{235}U = 6.235 x 10^{-4} at/barn, ^{238}U = 4.7205 x 10^{-2} at/barn);

(c) Hexagonal cells;

(d) Square cells.

CASE	EXPERIMENTAL VALUE	ENDF/B-II	ENDF/B-IV
BAPL-1	1.43 ± .01	1.3161 (-8.0)*	1.3334 (-6.7)
BAPL-2	1.15 ± .01	1.1208 (-2.5)	1.1349 (-1.3)
BAPL-3	.943 ± .010	.8466 (-9.4)	.8568 (-8.3)
TRX-1	1.320 ± .021	1.2696 (-3.8)	1.2915 (-2.2)
TRX-2	.837 ± .016	.7761 (-7.3)	.7870 (-5.9)

Table 4: Comparison of ρ^{28} calculated with the old and with the updated library.

(*): Values in brackets indicate the error in per cent of the experimental value.

CASE	EXPERIMENTAL VALUE	ENDF/B-II	ENDF/B-IV
BAPL-1	.089 ± .002	.0794 (-10.8)(*)	.0810 (-9.0)
BAPL-2	.072 ± .001	.0669 (-7.1)	.0679 (-5.7)
BAPL-3	.055 ± .001	.0498 (-9.5)	.0502 (-8.7)
TRX-1	.0987 ± .001	.0995 (.8)	.1032 (4.5)
TRX-2	.0614 ± .0008	.0606 (-1.3)	.0615 (.2)

Table 5: Comparison of δ^{25} calculated with the old and with the updated library.

(*): Values in brackets indicate the error in per cent of the experimental value.

CASE	EXPERIMENTAL VALUE	ENDF/B-II	ENDF/B-IV
BAPL-1	.078 ± .004	.0698 (-10.5)(*)	.0720 (-7.7)
BAPL-2	.070 ± .004	.0610 (-12.9)	.0631 (-9.9)
BAPL-3	.057 ± .003	.0478 (-16.1)	.0496 (-13.0)
TRX-1	.0946 ± .0041	.0889 (-6.0)	.0918 (-3.0)
TRX-2	.0693 ± .0035	.0594 (-14.3)	.0616 (-11.1)

Table 6: Comparison of δ^{28} calculated with the old and with the updated library.

(*): Values in brackets indicate the error in per cent of the experimental value.

CASE	EXPERIMENTAL VALUE	ENDF/B-II	ENDF/B-IV
BAPL-1	.8182 (a)	.7797 (-4.7)(*)	.7908 (-3.3)
BAPL-2	.7431 (a)	.7211 (-3.0)	.7307 (-1.7)
BAPL-3	.6614 (a)	.6365 (-3.8)	.6442 (-2.6)
TRX-1	.797 ± .008	.7661 (-3.9)	.7780 (-2.4)
TRX-2	.647 ± .006	.6188 (-4.4)	.6268 (-3.1)

Table 7: Comparison of C* calculated with the old and with the updated library.

(a): As no experimental values are available for these cases the reference values were obtained by means of the HAMMER code.

(*): Values in brackets indicate the error in per cent of the experimental value.

CASE	ENDF/B-II	ENDF/B-IV
TRX-1	1.0037	1.0047
TRX-2	1.0016	1.0025
BAPL-1	1.0001	.9996
BAPL-2	.9992	.9989
BAPL-3	.9962	.9944
YCE-1	1.0026	.9933
WAP-1	1.0060	1.0018
BAW-1	.9988	.9908
BAW-2	1.0488	1.0203
BAW-3	1.0589	1.0283

Table 8: Comparison of K_{ef} (for critical cells) calculated with the old and with the updated library.

[For captions of Table 9 and Figs V-1 to V-6 see lists at beginning of paper.]

```
ANGRA CELL (2.6 PC ENRCH.) INITIAL LOAD TEST PROBLEM NOVEMBER 1981
  1  0  0  0  0  1  1  0  0  0  0  0  0  1  0  0  0  1
            30.0          -0.41756     0.0          .110740
            60.0           0.0         .00154646    8.2421    -04
            70.0           0.0         3.40825   -031.81647   -03
           110.0           0.0         1.74966   -039.32410   -04
           991.0           0.0         0.0          0.0
          1000.0           0.0         .993076      .878075
          7770.0           0.0         0.0          0.0
           18-0.026
           291289.0
          7770.0
1200.       1250.          643.0       584.4        .737747   -04
.4095       .47491         1.2319        0.         0.           .0820313
2250.       0.             0.95
1.0         101.64                                                0.85
           1-150.          1289.
           2-850.          979.
           3-1000.         941.
           4-2000.         910.
           5-2000.         791.
           6-2000.         632.
           7-2000.         463.
           8-2000.         285.
           9-1000.         105.
          10-1000.         11.0
          7770.            0.
```

TABLE 9. Input data for the LEOPARD program, typical cell of Angra I, 10 degrees of burn-up

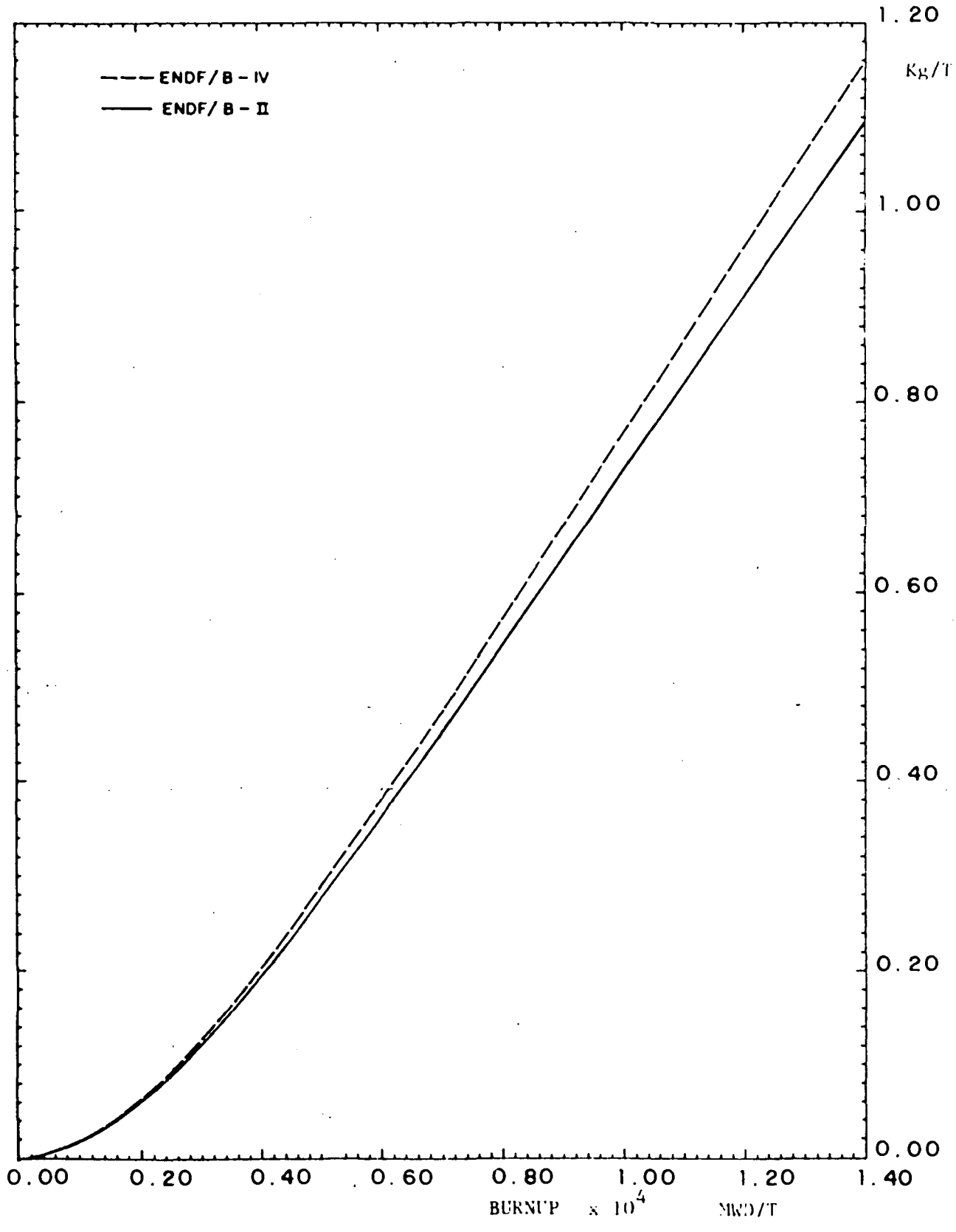

Fig. V-1. Rate of production of ^{240}Pu (kg/t) for various degrees of burn-up (MW·d/t)

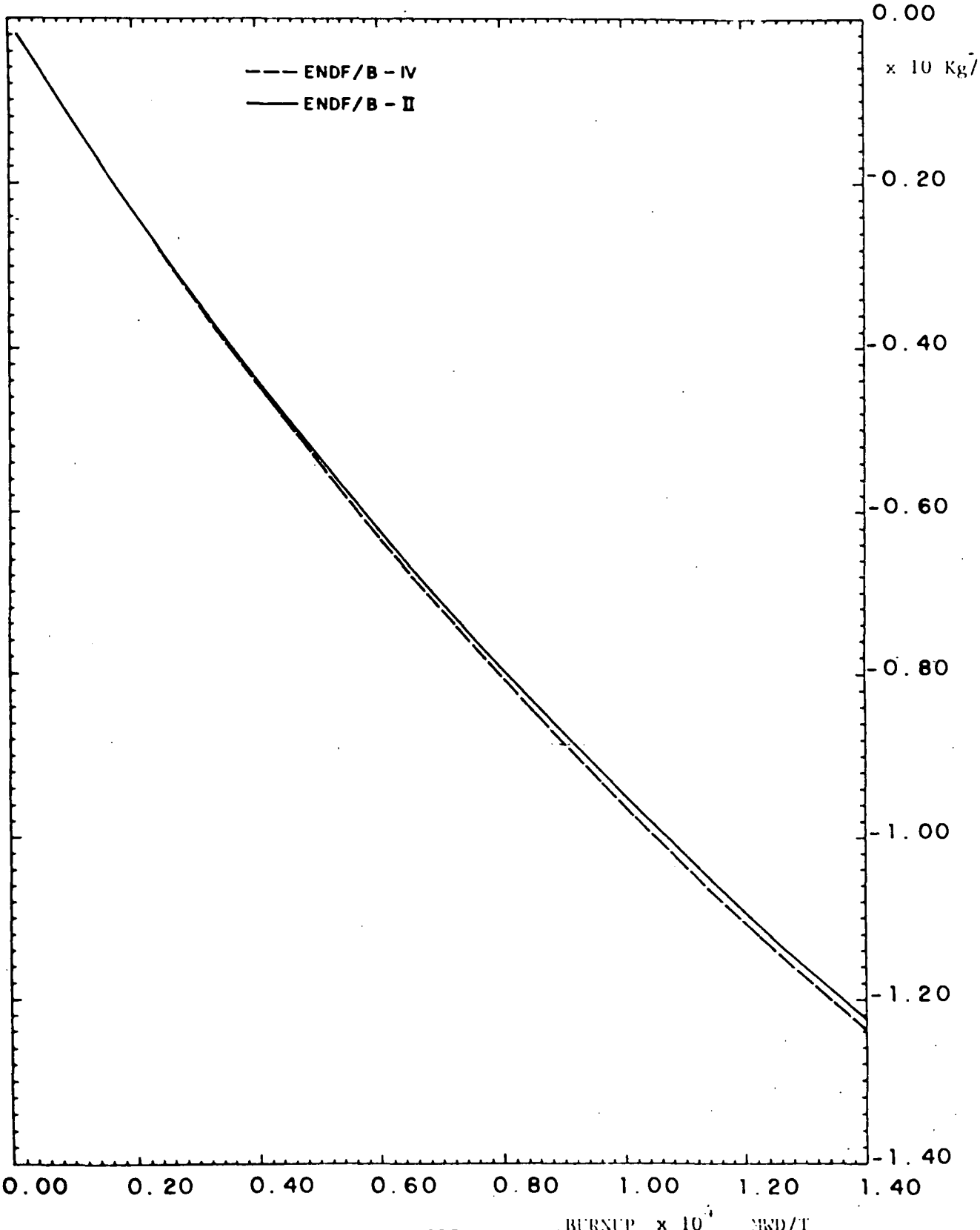

Fig. V-2. Rate of consumption of ^{235}U (kg/t) for various degrees of burn-up (MW·d/t)

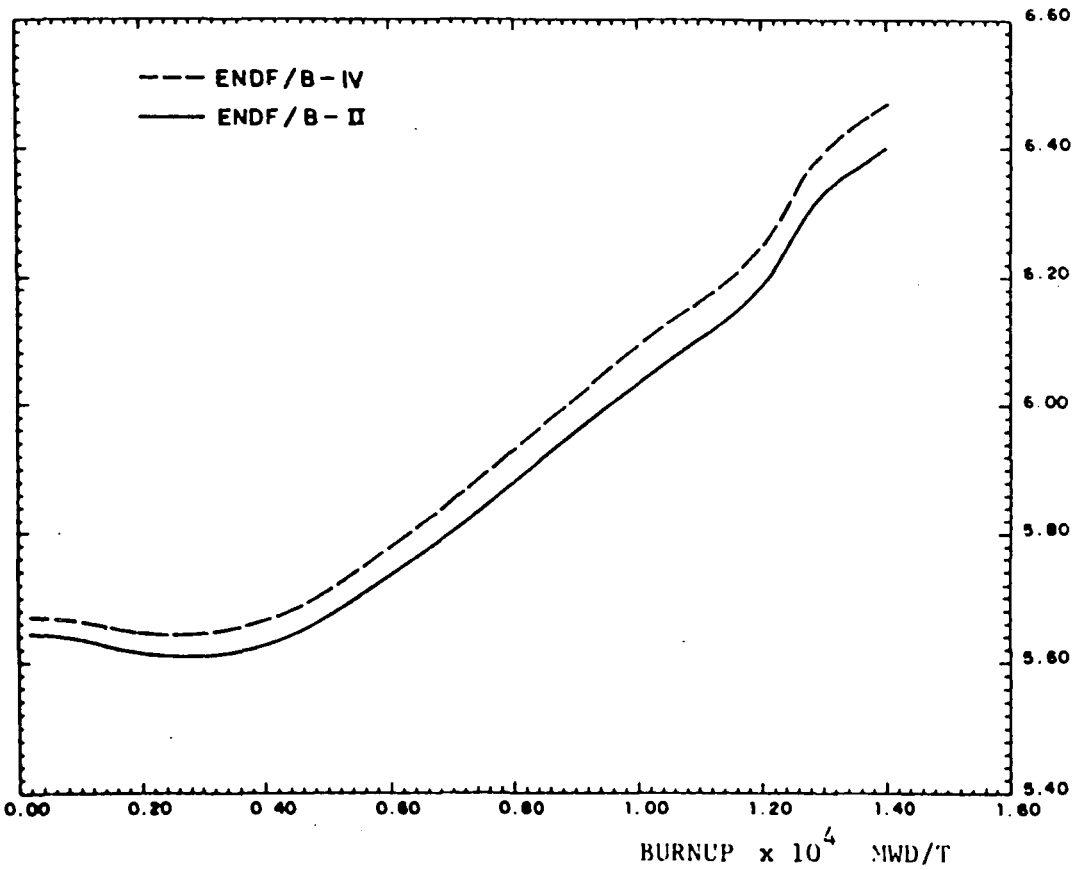

Fig. V-3. Rate of conversion (ratio between capture in fertile isotopes and absorption in fissile isotopes) for various degrees of burn-up (MW·d/t)

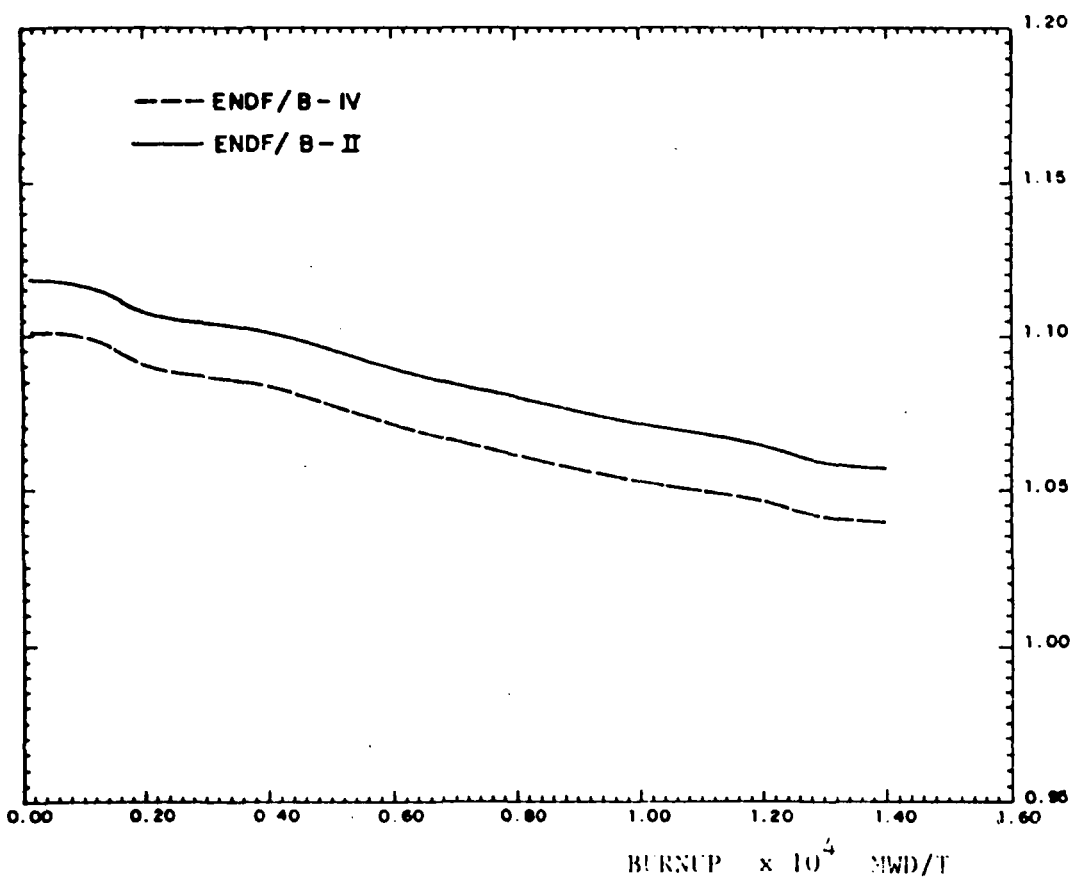

Fig. V-4. Infinite multiplication factor for various degrees of burn-up (MW·d/t)

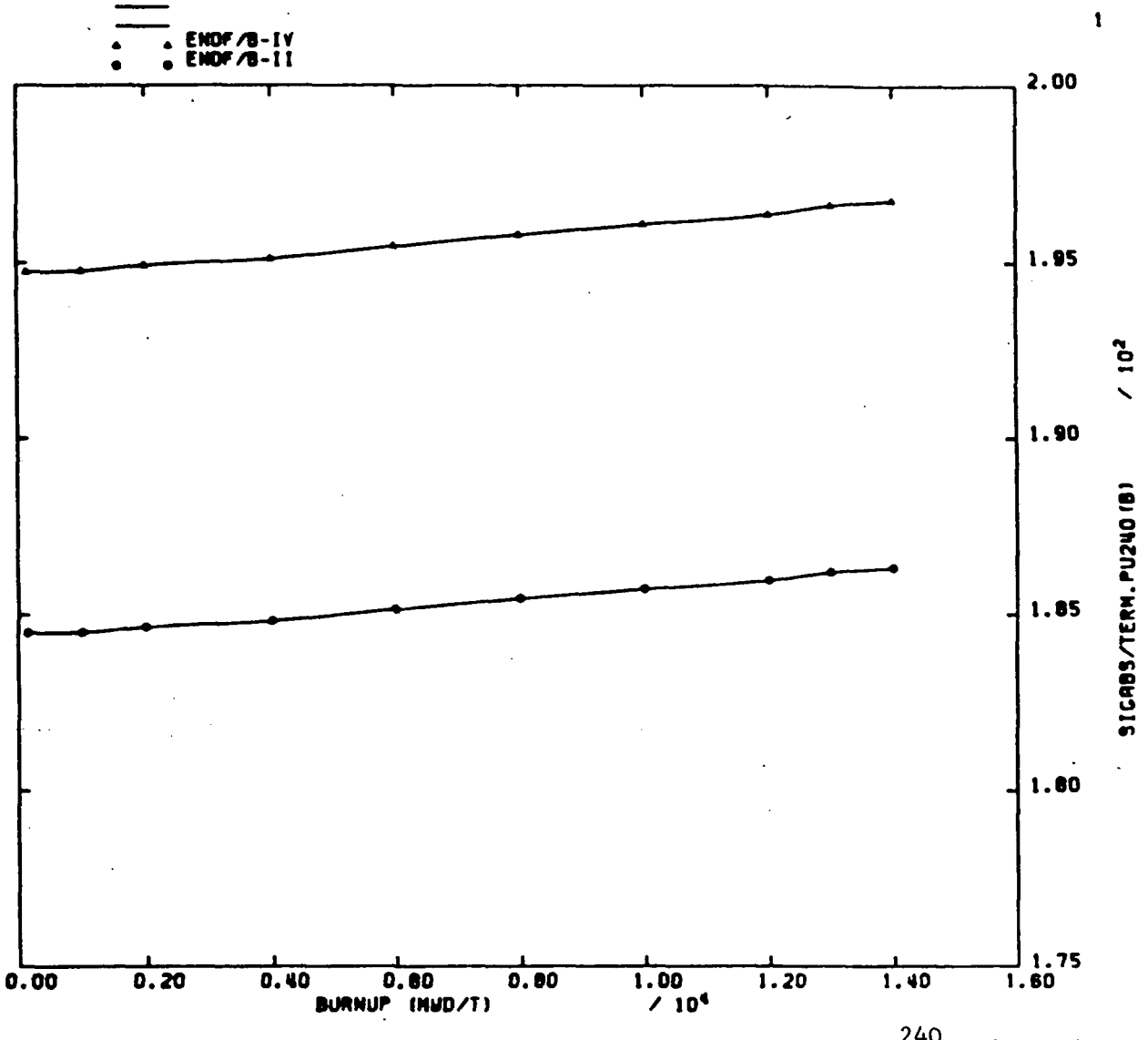

Fig. V-5. Microscopic thermal absorption cross-section of ^{240}Pu (barns) for various degrees of burn-up (MW·d/t)

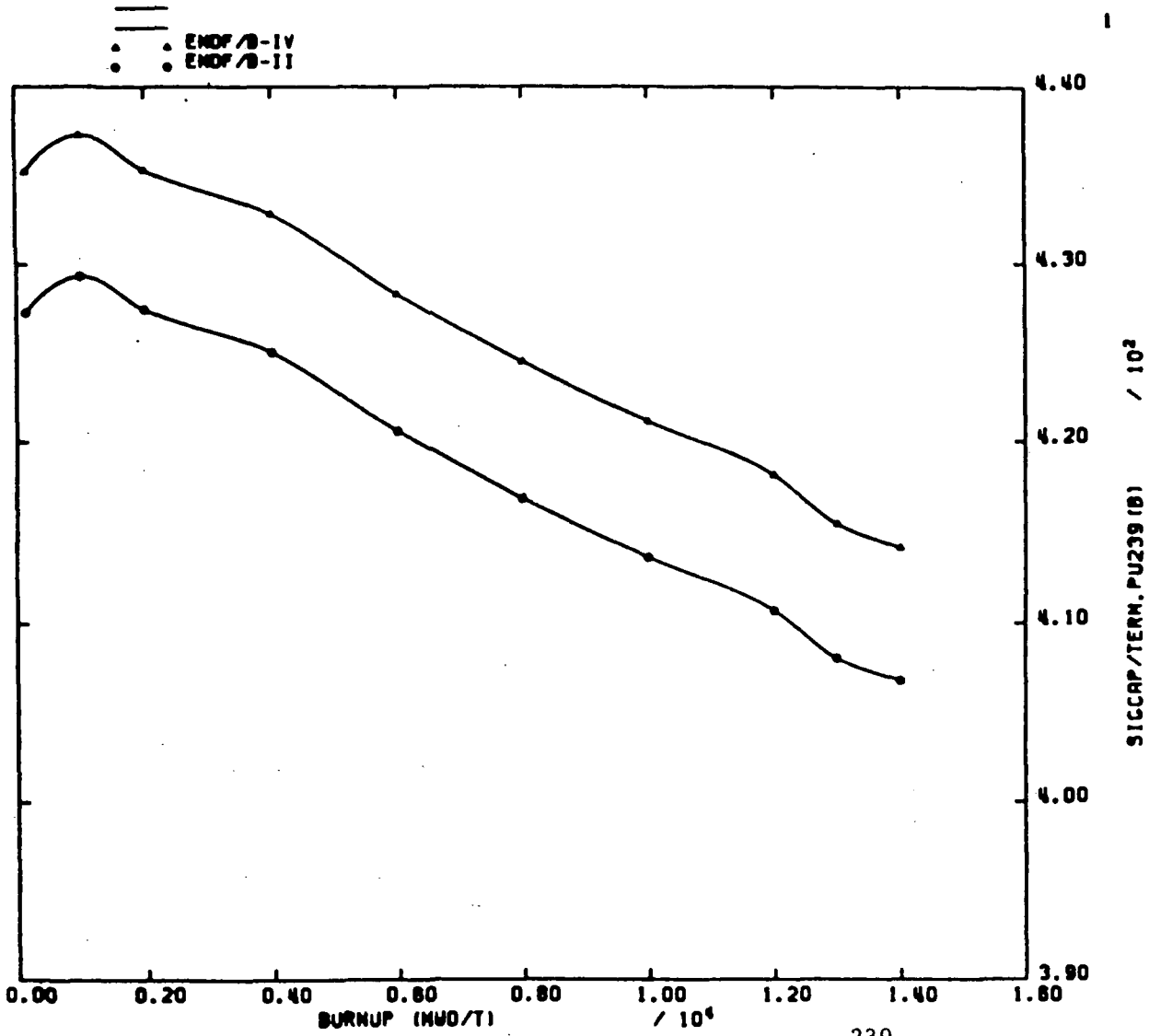

Fig. V-6. Microscopic thermal capture cross-section of ^{239}Pu (barns) for various degrees of burn-up (MW·d/t).