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ABSTRACT

Monte Carlo calculations were performed for estimating the perturbations in the activities of foils in a three-region fuel-cell due to the flux distorting effect of the foils themselves. Theoretical and numerical results show that the relative perturbations in the activaties of foils in both the fuel and moderator regions are nearly linear functions of the "absorption optical thicknesses" of the foils. The results are compared with estimates of other methods.

АННОТАЦИЯ

Методом Монте-Карло проведены расчеты возмущения активации фольг, вызванного наличием этих фольг в трехзонных твэлах. Теоретические и расчетные результаты показывают, что относительные возмущения активации как в топливе, так и в замедлителе, являются почти линейными функциями "толщины оптического поглощения" фольг. Результаты сравнены с другими опубликованными данными.

KIVONAT

Háromrégiós fütőelemcellába helyezett fóliák aktivációjában a fóliák jelenléte miatt fellépő perturbációt vizsgáltuk Monte Carlo módszerrel. Elméleti és numerikus eredmények arra mutatnak, hogy mind a fütőanyag, mind a moderátor régióban az aktivitás relativ perturbációja a fólia "abszorpciós optikai vastagságának" közel lineáris függvénye. Az eredményeket más módszerek becsléseivel vetettük egybe.

I. INTRODUCTION

Foil-activity measurements are frequently used in reactor physical experiments for the determination of neutron flux distributions and other reactor physical quantities. It is well known that the pure measured data suffer from a systematic error due to the presence of the foil in the measurements. This bias is the result of two phenomena: on one hand the absorption rate in the foil is usually different from that in the unperturbed system /in the system with no foil/ and this difference leads to the perturbation of the flux-distribution in the vicinity of the foil; on the other hand the altered absorption in the foil changes the number of neutrons that may travers several times the foil /i.e. the number of back-scattered neutrons/ and this change in the "self-shielding" results in a perturbation of the activity rate as compared to the theoretical activity, i.e. the integral of the activity cross section times the unperturbed flux.

A great number of theoretical considerations were presented for more or less idealistic cases /monoenergetic transport in infinite homogeneous medium with foil/ [1 - 4] . Although the results of these investigations provided good approximations to many realistic problems most of them are not able to account for positive perturbations while they may occure in case of foils with large scattering probabilities placed into fuel material. Furthermore these methods, being monoenergetic, are unable to take into account the effect of the energy spectrum on the perturbations. One more point is that a geometry so complex as an elementary cell with foils and with a cover region around the foil in the fuel /as in our case/ may not be considered homogeneous. /It will be seen, however, that for the foil in the moderator region the theoretical results may serve as a starting point for derivation of approximate analytical results./

In the following results obtained by Monte Carlo simulation

are presented for the cases of different foils in three-region fuel cells. In Section II the main features of the Monte Carlo program and the characteristics of the foils used in the calculations are reviewed. The calculated activity-perturbations are given in Section III. Theoretical considerations and fitting to the calculated values lead to approximate analytical expressions of the perturbations. These expressions are derived in Section IV. Discussion of the results and conclusions drawn from the calculations are summarized in Section V.

II. THE CALCULATIONS

II.1. The Monte Carlo program MOCAFO

The geometrical layout of the problem is given in Figure 1. The system consists of an infinitely long cylindrical fuel cell parallel to the /vertical/ z axis, composed of fuel, clad, and moderator regions. Identical horizontal foils are placed in the midplane of the moderator and of the fuel regions. The foil in the fuel is surrounded by a so called cover layer on both sides. A white boundary condition is assumed at the surface of the cell. For practical /statistical/ reasons reflective boundary conditions are prescribed at the horizontal planes situated at a distance of D from the midplane on both sides. This means that the foils are assumed to be placed periodically above each other with a period of 2D. According to experimental evidences[5] this periodicity has no sensible effect on the foil-activities if $D \geq 1$ cm. In the calculations D=2 was chosen.

The calculations were performed via correlated Monte Carlo method. In this method particles making their random walk account for the unperturbed and perturbed systems at a time. In other words there are several statistical weights assigned to a given particle, one of which is changed as if the particle were migrating in the unperturbed system, while the others are bound to reflect the effects of different perturbations to be taken into account.

The discussions of the correlated Monte Carlo technique would lead us too far from the subject and will be omitted here. The main consequence of the technique is that the unperturbed and perturbed results of a given calculation are in a strong correlation; in other words the random fluctuation among the parallel results are considerably decreased, the correlated results fluctuate together thus reflecting more accurately the tendencies in the correlated results. From technical point of view this technique allowed us to calculate several perturbed values in one run.

The calculations were performed in the energy region of [0.,0.625]eV, in 15 energy groups, corresponding to the group structure of the program THERMOS. The scattering was assumed to be linearly anisotropic in the LS, the absorption was taken into account by statistical weight reduction /survival biasing/. The necessary group constants, such as absorption and scattering cross sections, scattering matrices and average scattering angles, as well as the foil and cover activation cross sections were provided by the THERMOS code. The initial energy-spectrum of the starters was the one calculated from the 1/E scattering law again by the THERMOS code. The spatial distribution of the starters was uniform in the moderator /99.1% of the starters/ and in the fuel.

The program calculates the following quantities:

a./ Unperturbed results /in the absence of the foil/

- flux integrals in the sites of the foils /fuel, mod./

$$\Phi = \iint_{foil} \Phi_{unp}(\underset{\sim}{r}, E)\, d\underset{\sim}{r}\, dE \qquad (1)$$

-activation rates at the sites of the foils /fuel, mod./

$$A = \iint_{foil} \Sigma_{act}(E)\, \Phi_{unp}(\underset{\sim}{r}, E)\, d\underset{\sim}{r}\, dE \qquad (2)$$

- average fluxes /fuel, clad, moderator/

$$\bar{\Phi} = \Phi / V_{foil} \qquad (3)$$

b./ Perturbations due to the presence of the foils and cover /Perturbed values minus unperturbed values/
- perturbations in the foil activations /fuel, moderator/,
- perturbation in the cover activations /fuel/

As much as five perturbed cases were calculated in one run, differing from each other in the thickness of the cover around the fuel-foil. The corresponding cover thicknesses /on both sides/ were 0., 0.005, 0.010, 0.015, and 0.020 cm. /The calculation of the cover-activity perturbations was implemented into the code for it be enable to determine perturbations in such measurements where the cover activities are of primary importance./

c./ External reaction rates. At a maximum five sets of external cross sections can be specified in the input and the corresponding /unperturbed/ reaction rates are calculated by the program.

In order to check the program and the input data characterizing the cell, the average flux values /Eqs(1) and (3)/were compared. The number densities of the regions and the calculated values are listed in Tables I and II, respectively.

TABLE I

Number densities of the mixture elements in the calculated cells /in 10^{24} atom/cm^3/

Element	fuel	clad	moderator
H-1			6.671-2
O-16	4.589-2		3.336-2
Zr-40		3.868-2	
U-235	8.255-4		
U-238	2.210-2		

TABLE II

Average fluxes, $\bar{\phi}$, and velocities, $\bar{v}$, in the cell regions

	MOCAFO		THERMOS	
	$\bar{\phi}$	$\bar{v}$	$\bar{\phi}$	$\bar{v}$
Fuel	5.371±0.075	1.55±0.04	5.385	1.58
Clad	5.773±0.090		5.827	
Moderator	6.155±0.087	1.48±0.04	6.212	1.49

The program was written in FORTRAN with some routine programmed in assambler language of the PDP 11/10 computer.

II.2. Characteristics of the foils

Perturbations due to seven different foils were calculated by the program. The data characteristic of the foils are given in Table III. The average absorption and scattering cross sections were calculated by the program via the relation

$$\bar{\Sigma}_x = \int_R \int \Sigma_x(E)\,\phi_u(\underset{\sim}{r},E)\,dE\,d\underset{\sim}{r} \Big/ \int_R \int \phi_u(\underset{\sim}{r},E)\,dE\,d\underset{\sim}{r} \qquad (4)$$

where $\underline{x}$ stands for $\underline{a}$ /absorption/ or $\underline{s}$ /scattering/, while R refers to the region /fuel or moderator/. In the table N is the number density of the foil in 10^{24} atom/cm^3 and $\underline{d}$ is its thickness in cm.

TABLE III

Foils in the calculations

Foil	N	d	$\delta = \bar{\Sigma}_a d$		$\bar{\Sigma}_s$
			mod	fuel	
In-155	5.85-5	0.01	8.79-5	8.45-5	1.6-4
Mn-55/1/	3.1617-3	0.01	2.83-4	2.67-4	7.23-3
Dy-164	1.46-4	0.01	2.35-3	2.21-3	5.7-2
Cu-nat	8.496-2	0.01	2.56-3	2.42-3	0.6117
U-235	1.264-3	0.007	3.87-3	3.65-3	2.07-2
Mn-55/2/	7.6-2	0.01	6.80-3	6.41-3	0.1748
Pu-239	1.242-3	0.007	9.94-3	9.81-3	1.39-2

In case of U-235 and Pu-239 foils the fission rate represented the activity, in all other cases the absorption rates and their perturbations were calculated.

In all calculations the cover region was filled with Al of a number density 4.293-2. The foils as well as the cover were assumed to be pure one-component material with diagonal scattering matrices.

III. CALCULATED PERTURBATIONS

In Tables IV and V the calculated activity perturbations, relative to the unperturbed activity values are given in per cents /columns headed by P/ at the five different cover thicknesses /d_{Al}, in cm/; along with the relative standard deviations / σ /. To be more specific, let A and ΔA be the unperturbed activity /Eq.(2)/ and the perturbation in the activation, respectively. Then

$$p = \Delta A/A$$

and

$$P = 100.p \ [\%] \ .$$

Furthermore, let σ_1 and σ_2 be the standard deviations corresponding to A and ΔA, respectively. The standard deviation of P can be approximated as [6]

$$\sigma = P\sqrt{\left(\frac{\sigma_1}{A}\right)^2 - 2\varrho\frac{\sigma_1}{A}\frac{\sigma_2}{\Delta A} + \left(\frac{\sigma_2}{\Delta A}\right)^2} = 100\,\frac{\sqrt{\sigma_1^2 p^2 - 2\varrho\sigma_1\sigma_2 p + \sigma_2^2}}{A}$$

where ϱ is the correlation coefficient of A and ΔA. Now, since usually $p \ll 1$ and $\sigma_1 \lesssim \sigma_2$, the standard deviation becomes

$$\sigma = 100\,\frac{\sigma_2}{A}\,[1 - \mathcal{O}(p)] \approx 100\,\frac{\sigma_2}{A} \ [\%]$$

For each foils a linear regression calculation was performed to yield the line

$$P(d_{Al}) = P_o + m.d_{Al} \qquad (5)$$

TABLE IV. Relative perturbations in the moderator-foil at different cover thicknesses [%]

d_{Al} / Foil	0.000		0.005		0.010		0.015		0.020		P_o	m	A	σ_1
	P	σ	P	σ	P	σ	P	σ	P	σ				
In-155	-0.32	0.61	-0.26	0.62	0.11	0.64	0.47	0.65	0.78	0.66	-0.43	58.6	2.891-4	7.8-7
Mn-55/1/	-0.52	0.77	-0.23	0.78	0.21	0.81	0.36	0.80	0.64	0.81	-0.49	58.2	1.331-3	4.0-6
Dy-164	-2.21	0.61	-2.10	0.60	-1.79	0.61	-1.42	0.63	-1.10	0.64	-2.13	67.0	1.107-2	3.0-5
Cu-nat	-1.99	0.61	-1.94	0.64	-1.54	0.66	-1.09	0.67	-0.74	0.69	-2.30	58.0	1.200-2	4.0-5
U-235	-3.25	0.48	-2.98	0.49	-2.69	0.50	-2.33	0.51	-1.98	0.52	-3.28	63.8	1.553-2	3.0-5
Mn-55/2/	-4.24	0.58	-4.31	0.58	-3.82	0.59	-3.56	0.60	-3.12	0.62	-4.41	60.2	3.200-2	1.0-4
Pu-239	-5.73	0.27	-5.50	0.28	-5.22	0.28	-4.98	0.29	-4.73	0.30	-5.74	50.4	3.050-2	5.5-5

TABLE V. Relative perturbations in the fuel-foils at different cover thicknesses [%]

d_{Al} / Foil	0.000		0.005		0.010		0.015		0.020		P_o	m	A	σ_1
	P	σ	P	σ	P	σ	P	σ	P	σ				
In-155	1.13	0.38	1.62	0.48	2.70	0.55	3.52	0.60	4.35	0.64	1.24	166.4	1.436-4	3.6-7
Mn-55/1/	1.11	0.63	2.20	0.77	2.99	0.86	3.68	0.84	4.53	0.90	1.00	166.8	6.497-4	1.8-6
Dy-164	0.68	0.35	1.70	0.44	2.80	0.52	3.51	0.57	4.66	0.62	0.72	195.4	5.350-3	1.3-5
Cu-nat	0.10	0.38	1.39	0.52	2.60	0.61	4.13	0.67	5.27	0.72	0.08	261.6	5.843-3	1.8-5
U-235	-0.99	0.27	0.18	0.35	1.12	0.42	2.01	0.49	2.99	0.53	-0.90	195.8	7.500-3	1.8-5
Mn-55/2/	-2.39	0.38	-0.82	0.43	0.46	0.51	1.18	0.57	1.95	0.62	-2.06	213.6	1.551-2	4.5-5
Pu-239	-4.67	0.27	-3.88	0.30	-3.13	0.33	-2.32	0.35	-1.79	0.37	-4.63	147.6	1.551-2	3.2-5

best fitting to the perturbation values as a function of the cover thickness. The columns headed by P_o and m contain the fitted parameters of Eq.(5). In the last two columns of the tables the unperturbed foil-acticity-rates /A in Eq.(3)/ and their standard deviations / σ_1 / are listed that correspond to the average flux values given in Table II.

In Figure 2. the extrapolated zero-cover perturbation values /P_o/ are presented, as calculated by linear regression, as functions of the "differential absorption optical thicknesses":

$$\Delta_f = (\bar{\Sigma}_a^{foil} - \bar{\Sigma}_a^{fuel}) . d \ , \quad (\bar{\Sigma}_a^{fuel} = 0.3783)$$

/upper scale/ and

$$\Delta_m = (\bar{\Sigma}_a^{foil} - \bar{\Sigma}_a^{mod}) . d \ , \quad (\bar{\Sigma}_a^{mod} = 1.47\text{-}2)$$

/lower scale/. Triangles denote the mean values belonging to the foils in the fuel and to the upper scale, while circles represent the mean perturbations in the moderator-foil, plotted according to the lower scale. The bars around the mean values refer to the standard deviations. The scale used in the figure was proposed in ref.7 , where it was suggested that the perturbations are linear functions of Δ.

IV. THEORETICAL CONSIDERATIONS AND APPROXIMATE ANALYTICAL EXPRESSIONS

As it was stated in the introduction the analytical results derived theoretically for simplified cases are not expected to be applicable in their original form for our case. As a first approximations, however, one can assume that the foil in the moderator and the surrounding moderator region /i.e. the fluxes there/ are uneffected by the presence of the fuel region and the cladding. Accepting this assumption approximate expressions of the perturbation of the moderator-foil-activity can be derived from the infinite-foil, one group results. The effect of the fuel region

can be accounted for by appropriate choice of the parameters in the formula. The derivation, as given below, yields a rule of thumb for offhand approximate calculations of the perturbations.

According to ref.2 the relative perturbation in the aforementioned idealized case reads

$$P^* = \frac{(1+\varepsilon)\,\varphi(\delta)}{2\delta\,[1+g\,\varphi(\delta)]} - 1 \qquad (6a)$$

where

$$\delta = \bar{\Sigma}_a^{foil} \cdot d$$

$$\varphi(\delta) = 1 - 2E_3(\delta)$$

$$\varepsilon = \frac{2\delta}{\varphi(\delta)} \frac{d}{\pi R} \left(1 - \frac{\pi}{6}\delta\right) \qquad (6b)$$

and

$$g = \frac{1}{4}\sqrt{\frac{3}{1-c}}\left(1 - e^{-0.85R/L}\right) \qquad (6c)$$

Here c is the average number of secondaries in the moderator, i.e.

$$c = \bar{\Sigma}_s^{mod} / \bar{\Sigma}_t^{mod} ,$$

R is the radius of the cylindrical foil and L is the diffusion length in the moderator. In our cases $\delta \ll 1$, $R = \infty$ /white boundary condition/ and neglecting the powers of δ higher than three Eq.(6) becomes

$$P^* = -\frac{\delta}{2} \frac{(1-2\delta g)(B - \ln\delta) + 4g}{1+\delta g[2 - \delta(B - \ln\delta)]} \qquad (7)$$

with $B = 1 + \frac{1}{2} - \gamma = 0.92278$, γ being the Euler number. Furthermore $c = 0.994$ and thus $g = 5.6$. We have tried to reproduce our moderator-foil results in the form

$$P = P^* - a \quad , \qquad (8)$$

by fitting the values of $\underline{g}$ in Eq.(7) and $\underline{a}$ in Eq.(8). The fitted curve is given in Fig.2 by dashed line, the fitted parameters are

$$g = 1.7 \quad \text{and} \quad a = 0.3\ [\%]$$

Note that this value of $\underline{g}$ corresponds to an average number of secondaries in the moderator of c = 0.935. It is concluded that the decreased value of $\underline{g}$ as well as the presence of the additive constant $\underline{a}$ in Eq.(8) reflect the effect of the fuel region and the energy-dependent treatment for the following two reasons:

- the effective average number of the secondaries in the moderator is smaller than that in an infinite water medium since neutrons entering the fuel are removed from the system with a higher probability than those scattering in the moderator and therefore the number of neutrons being able to contribute to the moderator-foil-activity decreases,

- neutrons undergoing a scattering event in the foil do not loose energy, therefore the presence of the foil in energy-dependent calculations results in the hardening of the neutron spectrum. As the activity cross sections are decreasing functions of the energy the spectrum hardening leads to an additive negative activity-perturbation.

In fact Monte Carlo calculations show that even if the foil is purely scatterer /$\delta = 0$/ whilst its scattering matrix is diagonal a negative perturbation of the order of -0.3% is detected.

It is to be emphasized that the above considerations apply to the foil in the moderator region only and no similar results could be obtained for the fuel-foil.

As it is apparent from Fig.2 the perturbations are nearly linear functions of Δ ; the best fitting linear approximations to the calculated values are plotted in continous lines in Fig. 2. /The dysprosium perturbations - showing a systematic alteration from the assumed linear dependence - were omitted from the fitting./ The approximate linear expressions read

$$P_x = \pi_x + \mu_x \Delta_x \ , \quad / x = m, f / \qquad (9)$$

with

$$\pi_m = -0.82 \pm 0.21 \qquad \mu_m = -511. \pm 26. \qquad (10)$$

$$\pi_f = -0.69 \pm 0.13 \qquad \mu_f = -540. \pm 30. \qquad (11)$$

V. DISCUSSION AND CONCLUSIONS

A closer examination of the calculational results reveals some interesting tendencies.

As for the dependence of the perturbations on the cover-thickness it is apparent from Table IV that the slopes /m/ of the lines describing the dependence are very similar in magnitude for the foils in the moderator; i.e. the perturbations vary almost identically for every foil-material with an average slope of m ≐ 60. On the other hand the effect of the cover in the fuel region is surprisingly large on the activity of the moderator-foil. This relatively high sensitivity is very likely due to the fact that white boundary condition was assumed at the cell boundary. Another consequence of the white boundary condition is that the perturbations are overestimated to a certain extent; this overestimation can be approximately evaluated by comparing the approximated perturbation values calculated on the basis of Eqs(6) -(8)with $R = \infty$ and $R = 0.6668$ cm. In this latter case

$$g = 1.7(1 - e^{-0.85R/L}) = 0.563$$

where the factor 1.7 is the value of g as fitted for the case of $R = \infty$ and the diffusion length in the cell was chosen as $L = 1.41$.

The calculated values are given in Table VI for the different foils in the moderator. Note that in most cases the main difference between the infinite- and finite-foil results is due to the drastic change in the value of g /the value of which may be rather doubious for the great number of approximations/, while the edge-correction, ε, is about 0.47% and 0.33% for the foils

of thicknesses 0.01 and 0.007 cm, respectively.

The approximate results in Table VI must be accepted with a certain reservation and the differences between the finite- and infinite-foil perturbations are very likely exaggerated as it will be pointed out below in connection with a comparison of our results with other /Monte Carlo/ calculations.

TABLE VI

Approximate theoretical activity-perturbations /in%/ in the moderator -foils of different radii R

Foil \ R	∞	0.6668
In-155	-0.37	+0.12
Mn-55/1/	-0.52	0.
Dy-164	-1.90	-0.91
Cu-nat	-2.03	-1.00
U-235	-2.82	-1.65
Mn-55/2/	-4.48	-2.57
Pu-239	-6.14	-3.78

In order to check the real effect of the white boundary condition on the perturbation as well as the quality of the approximate corrected values of Table VI Monte Carlo calculations were performed where it was assumed that a particle leaving the cell will never return and a new particle /never having been in the cell/ enters the cell instead of that having left. /"Selective white boundary condition"/ These results, however, show much higher deviations from the real perturbations /in the opposite direction/ than those given by white boundary condition.

The dependence of the fuel-foil perturbations on the cover thickness is much less regular than that in the case of the moderator-foils. The slopes of the fitted lines in Table V are

very different. It is remarkable that the highest m-value, alike in the case of the moderator-foil, belongs to the Cu-foil. As the most outstanding difference of this foil from all the others is its very large scattering cross section /see Table III/ it is felt that the high value of $\underline{m}$ is a consequence of the pronounced scattering in the foil.

It is apparent from Fig.2 that none of theperturbations is zero when the foils are identical with the surrounding material /moderator or fuel/. One reason for this was found in the spectrum hardening effect of the foils, as discussed in the previous section. The most important motive behind it lies, however, in the interaction of the perturbations. In other words, even if the foil is identical with one of the surrounding regions it perturbs the neutron field in the other and this perturbation propagates into the otherwise unperturbed region thus yielding an activation perturbation also there.

According to Eqs(9) - (11) the perturbations in the moderator and fuel foils, as functions of the "differential absorption optical thickness" have very similar slopes, i.e. the difference of the perturbations in the two regions is essentially constant. Moreover Π_m and Π_f, the constant terms in the linear approximations to the perturbations do not differ significantly from each other and one is tempted to believe that the perturbations depend only on the "differential absorption optical thickness", irrespective of the surroundings. This conjecture, however is not sufficiently justified by evidences.

Previous /Monte Carlo/ calculations by Maiorov [8] may be compared to the present results. The perturbations presented in ref.8 and the corresponding results of ours are summarized in Table VII for different foils and Al cover thicknesses. The calculations of ref.8 were performed for foils in hexagonal cells situated in a hexagonal lattice. In the lattice every 8th cell con-

tained foils and it is reasonable to assume that the foils were far enough from each other for not to interact.

TABLE VII

Comparison of foil perturbations

Foil	d_{Al}	in mod.		in fuel	
		ref.8	present	ref.8	present
Mn-55/2/	0.00	-3.39±0.8	-4.25±0.58	-2.05±1.0	-2.39±0.38
U-235	0.02	-2.34±0.8	-1.98±0.52	3.53±0.8	2.99±0.53
Pu-239	0.00	-5.84±1.0	-5.73±0.27	-0.59±1.1	-4.67±0.27
Pu-239	0.02	-4.83±1.0	-4.73±0.30	1.37±1.1	-1.79±0.37

The very good agreement between the different calculations indicate that the white boundary condition /i.e. the implicite assumption of an infinite foil/ does not lead to so strong deviation from the realistic case as it is predicted in Table VI. /We believe that the drastic disagreement in the -Pu- foil data is accidental./

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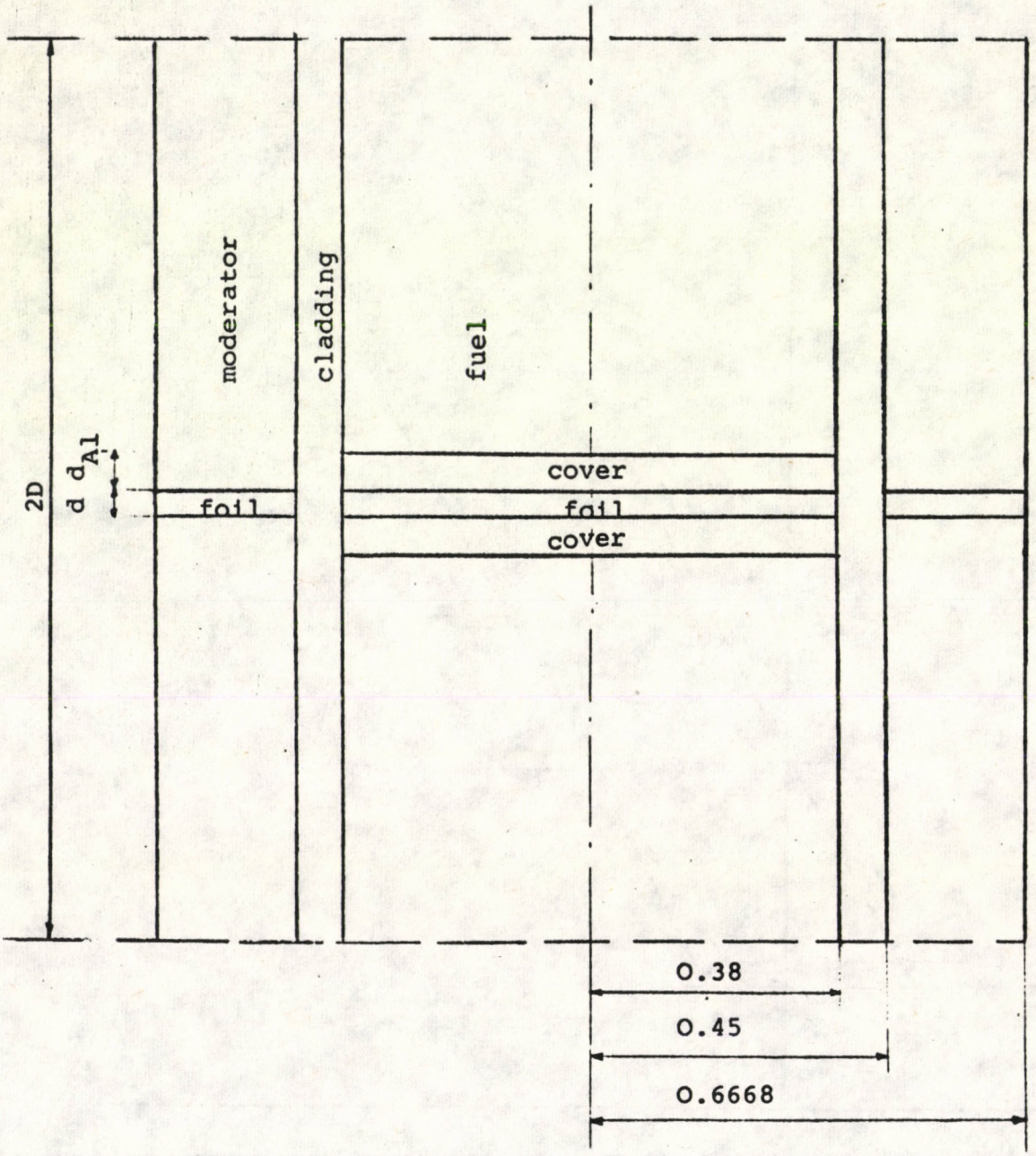

2D
d
d_{Al}
moderator
cladding
fuel
foil
cover
foil
cover
0.38
0.45
0.6668

Figure 1.

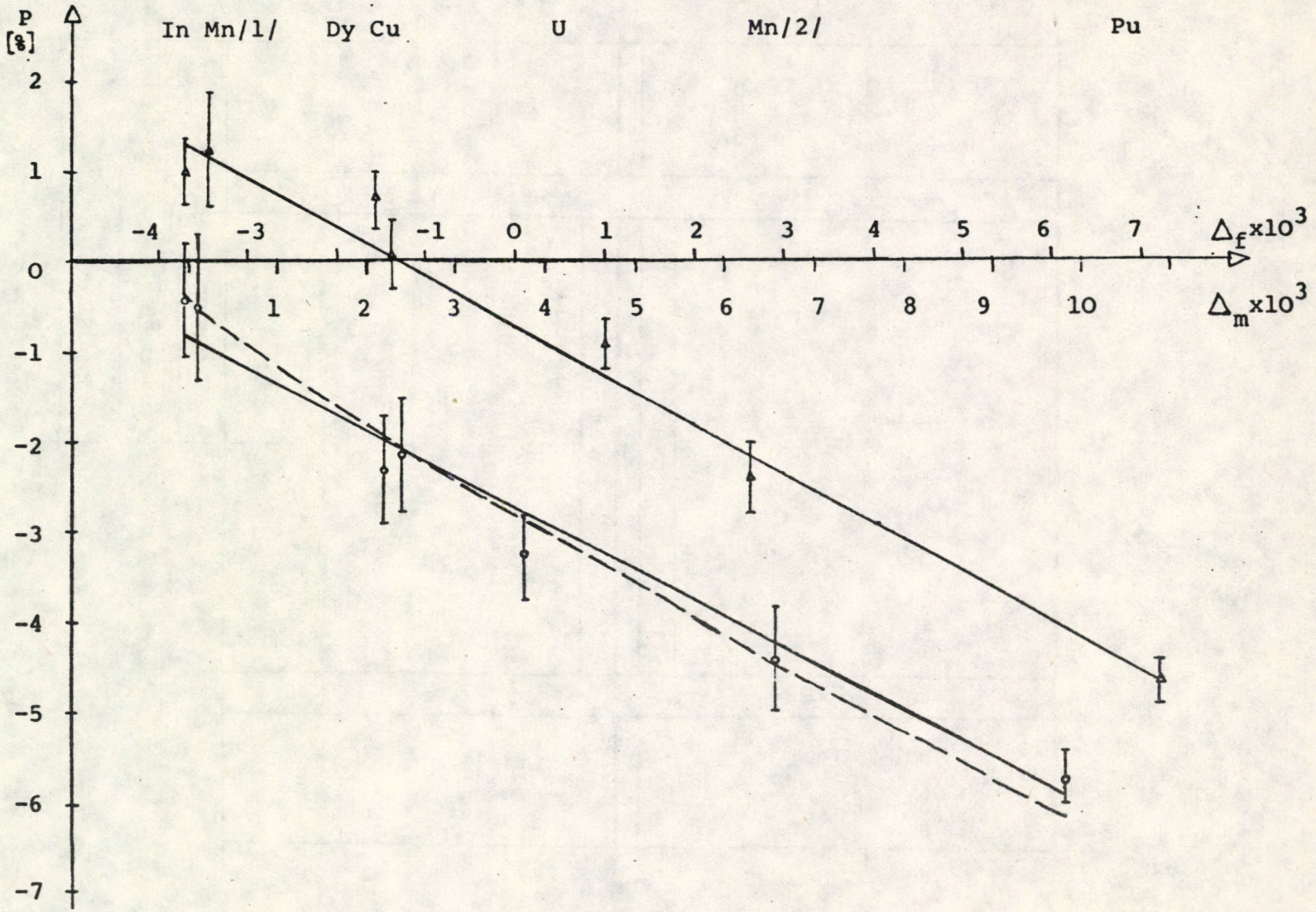
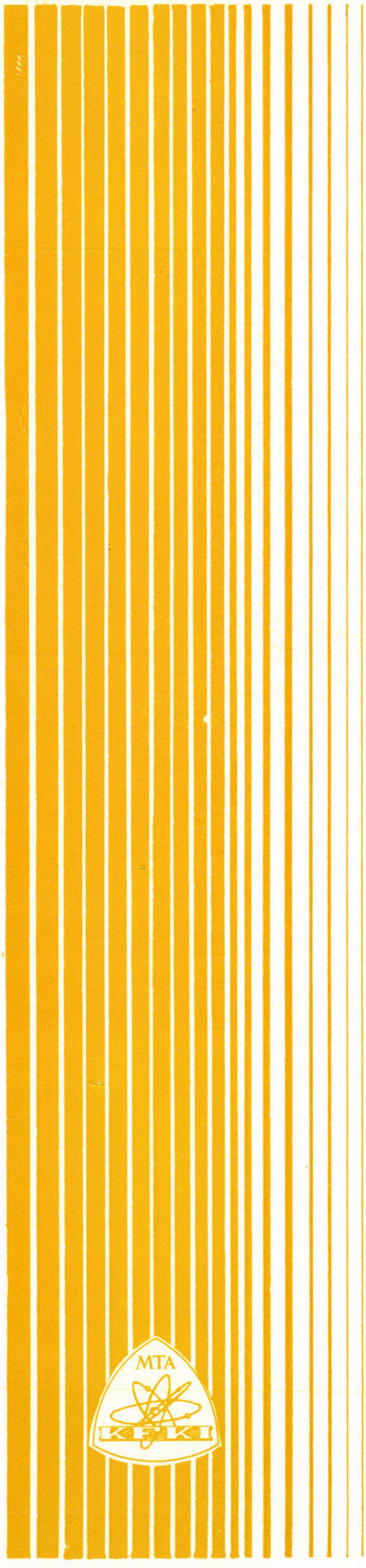

P [%]
In Mn/1/
Dy Cu
U
Mn/2/
Pu
2
1
0
-1
-2
-3
-4
-5
-6
-7
-4
-3
-1
0
1
2
3
4
5
6
7
$\Delta_f x10^3$
1
2
3
4
5
6
7
8
9
10
$\Delta_m x10^3$

Figure 2.



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Gyimesi Zoltán
Szakmai lektor: Gadó János
Nyelvi lektor: Pázsit Imre
Példányszám: 310 Törzsszám: 81-305
Készült a KFKI sokszorosító üzemében
Felelős vezető: Nagy Károly
Budapest, 1981. május hó