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Institut für Neutronenphysik und Reaktortechnik

Projekt Schneller Brüter

Check of Nuclear Data and Methods of Calculation by Integral Experiments

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Gesellschaft für Kernforschung m.b.H., Karlsruhe

Abstract

In this work we are dealing mainly with calculations concerning integral experiments in fast zero power assemblies. By comparing calculated and measured quantities we want to check the nuclear data and methods of calculations used and try to get indications for further improvements. Following a few introductory remarks some comments to the state of the art of the physics prediction for fast reactors are given. Then the activities at Karlsruhe to improve the nuclear data and methods of calculation, especially some of the most recent results, are described. At first the improvements in the group constant sets are considered and the influence of the energy dependence of the fission spectrum is studied. It is outlined that the proper treatment of relatively thin reflecting zones is difficult in the present scheme of calculations even if a more appropriate type of transport cross section is used. For the SUAK-assemblies the influence of an uncertainty in the enrichment on the criticality is determined. The criticality effect of using the P1-approximation for the scattering on hydrogen instead of the transport approximation is studied for SUAK UH1B and SNEAK 3A2.
The difficulties concerned in the calculation of material worths and neutron life time are discussed. The theoretical results obtained at Karlsruhe for the Doppler effect seem to be satisfactory at the moment. The influence of the model used for the calculation of reaction rates and cell traverses for heterogeneous platelet-arrangements is studied and the experimental and theoretical results for the cell traverses are compared. The measured and calculated reaction rate traverses through core and blanket of SNEAK 3A2 are also compared with special emphasis on heterogeneity effects in the core-blanket transition region.
In the Appendix some personal comments are devoted to the significance of adjustment procedures for group constants.

Zusammenfassung

In dieser Arbeit befassen wir uns mit der Nachrechnung integraler Experimente in schnellen Nullenergie-Anordnungen. Der Vergleich der berechneten mit den gemessenen Größen dient hauptsächlich der Überprüfung der Kerndaten und Berechnungsmethoden und soll Hinweise auf notwendige Verbesserungen liefern.
Nach einigen einleitenden Bemerkungen wird dargelegt, welchen Stand die reaktor-physikalischen Vorhersagen für schnelle Reaktoren erreicht haben. Danach werden die in Karlsruhe unternommenen Anstrengungen zur Verbesserung der nuklearen Daten und Rechenmethoden beschrieben und die jüngsten Ergebnisse aufgeführt. Die Verbesserungen in den Gruppenkonstantensätzen werden kurz erläutert und der Einfluß der Energieabhängigkeit des Spaltspektrums wird untersucht. Es wird dargelegt, daß eine angemessene Behandlung relativ dünner Reflektorzonen innerhalb des gegenwärtigen Berechnungsschemas schwierig ist. Die Benutzung eines geeigneteren Transportquerschnitts in den Transportrechnungen beseitigt nur einen Teil dieser Schwierigkeiten. Für die SUAK-Anordnungen wird der Einfluß einer Unsicherheit in der Anreicherung auf die Kritikalität bestimmt. Für SUAK UH1B und SNEAK 3A2 wird gezeigt, welche Auswirkungen auf die Kritikalität sich ergeben, wenn man statt der Transportnäherung die P1-Näherung für die Streuung an Wasserstoff benutzt.
Die Schwierigkeiten, die bei der Berechnung von Materialwerten und Neutronenlebensdauern auftreten, werden diskutiert. Bezüglich des Dopplerkoeffizienten kann festgestellt werden, daß die zur Zeit in Karlsruhe berechneten Werte eine zufriedenstellende Übereinstimmung mit den Experimenten aufweisen. Für den in schnellen Anordnungen üblichen heterogenen Plättchenaufbau wird untersucht, welche Auswirkungen das den Rechnungen zugrunde liegende vereinfachte Modell auf die Berechnung von Reaktionsraten und Zelltraversen besitzt. Die im Core und im Blanket von SNEAK 3A2 gemessenen Reaktionsratentraversen werden mit berechneten Ergebnissen verglichen, wobei besonders auf Heterogenitätseffekte in der Core-Blanket-Übergangszone geachtet wird.
Der Anhang enthält einige Bemerkungen und persönliche Ansichten über die Bedeutung der Gruppenkonstanten-Anpassung.

Contents

I. INTRODUCTION

One of the primary objectives of theoretical reactor physics is the prediction of the nuclear characteristics of power reactors. A high accuracy and reliability of this prediction for many important characteristics is necessary from the economic point of view as we know e.g. from the studies of GREEBLER and HUTCHINS [1], [2]. Economics are therefore the most important incentive to increase the accuracy and reliability of the nuclear data and the calculational methods and to check the theoretical results with corresponding experiments. Besides the economic incentive there is the natural scientific incentive which calls for explanations of the existing discrepancies between calculation and measurement and finally calls for improvements and refinements in theory and experiment to obtain agreement for corresponding results.

It is at present generally accepted that it is very difficult to create a satisfactory set of group constants for reactor calculations which is based on differential measurements only without using the results of integral experiments. Therefore, it is necessary to compare the experimental results of critical experiments with the results of calculations using the best available nuclear data and methods of calculation.

In chapter II some comments to the state of art of the physics prediction for fast reactors are given. The activities at Karlsruhe to improve the nuclear data and methods of calculation, especially some of the most recent results, are described in chapter III. At first the improvements in the group constant sets are considered (III.1) and the influence of the energy dependence of the fission spectrum is studied (III.2). It is outlined in III.3 that the proper treatment of relatively thin reflecting zones is difficult in the present scheme of calculations even if a more appropriate type of transport cross section is used (III.4). For the SUAK-assemblies the influence of an uncertainty in the enrichment on the criticality is mentioned in III.5. The criticality effect of using the P1-approximation for the scattering on hydrogen instead of the transport approximation is studied in III.6 for SUAK UH1B and SNEAK 3A2.

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The difficulties concerned in the calculation of material worths and neutron lifetime are discussed in III.7 and III.8 respectively. In III.9 we draw the conclusion that the theoretical results obtained at Karlsruhe for the Doppler effect seem to be satisfactory at the moment. The influence of the model used for the calculation of reaction rates and cell traverses for heterogeneous platelet-arrangements is studied in III.10 and the experimental and theoretical results for the cell traverses are compared in III.11. A comparison of the measured and calculated reaction rate traverses through core and blanket of SNEAK 3A2 is given in III.12.
In the Appendix some personal comments are devoted to the significance of adjustment procedures for group constants.

II. COMMENTS TO THE STATE OF THE ART

The most important quantity used in the comparison between theory and experiment is the criticality k_{eff} or the critical mass of the reactor system. Fig. 1 illustrates the situation in 1966 when DAVEY [3] compared the prediction for the assembly ZPR III-48 obtained by various groups working on fast reactor physics. It can be seen that the predictions of critical mass differ by up to 100 kg, a relatively large amount compared to the 272 kg really present in the experiment. The calculated central reaction rate ratio $\sigma_c(U238)/\sigma_f(U235)$ considered as a spectral index in [3] differs by about 10% between the extreme cases. The experimental result is beyond of all the theoretical results and even if the experimental value is decreased by 5%, according to the given experimental uncertainty of ±5%, most of the theoretical results still remain below the lowest value which seems to be acceptable from the point of view of the measurements. This indicates that most calculations lead to a systematic underprediction of the reaction rate ratio $\sigma_c(U238)/\sigma_f(U235)$. The probable reason is that in most sets of group constants a too low capture cross section of U238 was assumed at that time.

Fig. 2 shows the predictions for the central perturbation cross section of Na and for the central ratio $\sigma_c(U238)/\sigma_f(Pu239)$ derived from the

given ratios [3] $\sigma_c(U238)/\sigma_f(U235)$ and $\sigma_f(Pu239)/\sigma_f(U235)$. The first quantity can be considered as representative of the central sodium void coefficient, the second one gives an indication of the prediction of the breeding performance. Comparing the different results one should have in mind that they have not been derived for identical reactors because the different participants of this intercomparison have been asked to adjust the radius of the assembly in such a manner that criticality is achieved. Considering the very large discrepancies observed in Fig. 2, this fact, however, seems to be of minor importance.
For the sodium void coefficient a change of sign can even be found in one case and in several cases there is an overprediction by a factor of 2. For the breeding performance -or more precisely for the conversion ratio- a difference of about 20% can be observed between the two most extreme values.
This leads us to the conclusion that in 1966 the criticality was predictable with ±3%, the conversion ratio with ±10%, and such an important reaction rate ratio as $\sigma_c(U238)/\sigma_f(U235)$ also with ±10% of accuracy. The uncertainty attributed to the sodium void coefficient was ±100% at that time.
Fig. 3 is taken from an intercomparison too, which has been evaluated by BAKER [4] in 1969. The reactor considered here is a simplified model of a 1000 MWe sodium cooled fast reactor. All groups participating in this intercomparison had to adjust the enrichment appropriately so that criticality was achieved for a given geometry. From Fig. 3 it can be seen that the breeding gain for these critical reactors differs by about 0.17 between the most extreme results. This difference of about 50% for such an important quantity is amazing having in mind that this will cause an uncertainty of the doubling time by about the same amount. The k_{eff}-values of Fig. 3 were determined by the group which performed the evaluation for this intercomparison using additional information provided by the various participants. The composition obtained for the Winfrith FD4 calculation was used as the basis for this k_{eff}-estimate for identical reactors. Therefore, the Winfrith FD4-k_{eff} value is unity just by definition because it is the reference point.
Compared to the situation in 1966, the improvement obtained up to 1969 in the physics prediction seems to be rather small. The uncertainty in k_{eff} is still large, about ±2.5%, although most of the results are within a ±1% uncertainty range. There is still a ±25% uncertainty in the breeding

gain equivalent to a ±7% uncertainty in the breeding ratio which has to be compared with the ±10% uncertainty in the conversion ratio observed in 1966.

These facts demonstrate that the physics prediction of fast reactor characteristics cannot be considered as satisfactory at present. Further efforts are necessary to reach the goal of sufficiently accurate physics prediction for the future economic large fast power reactors.

Mock-ups for these reactors are presently built in the United States. Because of their large size they are rather expensive. Although they provide valuable additional information it may be questionable whether they are justified or necessary from an economic point of view, especially if one takes into account that they provide only few information on long term behavior and safety characteristics as e.g. power transients. Therefor it may happen that at least in Europe the design of large fast power reactors has to rely to a large extent on theoretical predictions which, of course, are based on extensive checks for a variety of smaller and not so expensive assemblies. This is the reason why a high accuracy for the theoretical results ultimately must be attained which implies continuous improvements of the nuclear data basis and of the methods of calculation and the check of both, methods and data, with integral experiments for which also a high accuracy and reliability has to be required.

As a concluding remark to this chapter it seems worthwhile to refer to the results obtained by FILLMORE et al. [5] who determined k_{eff} and other quantities for the same reactors using the same basic nuclear data but different procedures for the generation of group constants. The results partially given in the following table are not very encouraging.

Table 1

Comparison of results obtained for ZPR III-48 using the same nuclear data but different procedures for the generation of group constants: GRISM and MC^2

Quantity	$\frac{\text{GRISM-result}}{MC^2\text{-result}}$
k_{eff}	0.9925
F_{28}/F_{25}	0.953
C_{28}/F_{25}	1.06
MW U-238	1.12
MW Pu-240	0.89
MW Cr	1.69
MW Ni	1.27
MW Na	1.31

$\hat{MW}$ = material worth

Although it is quite certain that the differences of some of the quantities are due to the different methods of treating the resolved resonances by the two codes, the discrepancies observed here clearly indicate that besides improving the basic nuclear data it may be necessary to reconsider the methods used for the preparation of group constants. If the theoretical treatment adopted in these methods is not refined enough and if insufficient approximations are used one must expect a considerable degree of uncertainty in the generated group constants.

III.A. ACTIVITIES AT KARLSRUHE TO IMPROVE NUCLEAR DATA AND METHODS OF CALCULATION

III.1 Improvements in group-constant-sets

Before 1967 the well-known Russian ABN-Set [6] had been used mostly for the calculation of fast reactors at Karlsruhe. On the basis of the KEDAK-file, the evaluated nuclear data file established at Karlsruhe, first the KFK-Set [6a] and then the so-called SNEAK-Set [7], [8] were prepared which may be considered as improved versions of the ABN-Set. The first assembly calculated with this new SNEAK-Set was SNEAK-3A1 [9]. The agreement observed between theory and experiment for the criticality of this assembly was surprisingly good -the difference was about 0.5%-. It was therefore suspected that some adjustment had been performed. This was not the case; all nuclear data which were improved compared to the ABN-Set had been taken from the KEDAK-file. The only correspondence to the SNEAK-assembly consisted in the use of the spectrum of SNEAK-3A2 as a weighting spectrum for the generation of group constants. Subsequent studies [10] showed that this first good agreement between theory and experiment was to some extent fortuitous.

Further improvements resulted in the so-called MØXTØT-Set [11] which was presented at the 1969 BNES-Conference in London [12]. The assemblies chosen for a systematical check [11], [12] of the nuclear data and methods of calculation covered a broad range of different material and geometric compositions and resulted in rather different energy distributions of the neutron spectra. With the MØXTØT-Set we suceeded to predict the criticality of all assemblies considered in the study with a maximum deviation of ±2%.

Another important success of the MØXTØT-Set -also confirmed by more recent results- is the nearly clear cut between the criticality-deviations of U-235- and Pu-239-fuelled assemblies leading to the conclusions that U-235-+U-238-mixtures were predicted somewhat supercritical and Pu-239-+U-238-mixtures somewhat subcritical.

As could be expected the mixed fuelled assemblies SNEAK-3B2 and SNEAK-4A were predicted rather well because of compensation effects.

Because of the encouraging results obtained with the MØXTØT-Set, other assemblies have been calculated with this set of group constants too, e.g. the recently built SNEAK-4A, $k_{eff\ calc.}/k_{eff\ meas.}$ = 0.999 [13], SNEAK-2A, k_{eff} = 1.018 [14]. A recalculation of the well-known small assemblies showed the following results [15]: GODIVA (bare uranium-sphere) 1.016, TOPSY (uranium sphere, reflector: natural uranium) 1.020, JEZEBEL (bare plutonium sphere): 1.001, POPSY (plutonium sphere, reflector: natural uranium) 1.009. These results have been obtained by S_6-calculations using the transport approximation for the description of the scattering process. Using a higher S_N-order will reduce these results by about 0.5% [15] and a change of the description of the neutron scattering (e.g. P_3-approximation) may lead to further small changes for the theoretical criticality value but will not alter the main conclusions.

For VERA-11A a criticality value k_{eff} = 1.000 has been obtained. A possible error in this theoretical value is caused by the uncertainty in the rather large transport correction. By addition of our one-dimensional corrections: axial (S_{16}): 0.0204, radial (S_8): 0.0353 we obtained Δk (transport correction): 0.0557 whereas BAKER [16] e.g. reported a best S_4-value of 0.053 which could reduce to 0.043 if $S_{inf.}$ and a finer mesh size are accounted for.

These recently determined criticality values confirmed our previous experience of a maximum deviation of ±2% between measured and calculated criticality.

III.2 Influence of the fission spectrum

The standard fission spectrum used in our calculations in that belonging to ν=2.8 of the ABN-Set [6]. In [12] we studied the influence of the fission spectrum on criticality in a rough manner by applying the variations which are given in [6] for the dependence of the fission spectrum on the mean number of fission neutrons per

fission. The results were rather small changes

a) for criticality: a reduction of 0.001 - 0.003 for uranium fuelled assemblies and an increase of 0.001 for plutonium fuelled assemblies.

b) for the central fission ratio $\sigma_f(U238)/\sigma_f(U235)$: a reduction of 1.2% for uranium fuelled assemblies and an increase of 2% for plutonium fuelled assemblies.

FABRY [43] among others [44], [45] has obtained some indications from his measurements that the U235 thermal fission spectrum has to be modified compared to the previously generally used form. The influence of his preliminary results [46] has been studied for SNEAK-3A1 and SNEAK-3A2.

Table 2

Change caused by the introduction of FABRY'S fission spectrum

	k	$\frac{\sigma_f(U238)}{\sigma_f(U235)}$
SNEAK-3A1	+0.0023	+ 4.3%
SNEAK-3A2	+0.0019	+ 4.4%

For ZPR III-48 for the same change in the fission spectrum the following results have been obtained:

	k	$\frac{\sigma_f U238}{\sigma_f U235}$	$\frac{\sigma_f Pu240}{\sigma_f U235}$	$\frac{\sigma_f Pu239}{\sigma_f U235}$	$\frac{\sigma_c U238}{\sigma_f U235}$	$\frac{\sigma_c Pu239}{\sigma_f Pu239}$
ZPRIII-48	+0.0035	+4.5%	+1.8%	+0.25%	-0.25%	-0.6%

These results indicate that although there is a certain increase in the central fission ratio $\sigma_f(U238)/\sigma_f(U235)$ this effect is not large enough to explain our present discrepancy for this quantity. Therefore this fact is a further strong indication that the inelastic scattering cross section for U238 has to be reduced in the high energy range above about 1 MeV to get an improved agreement

between theory and experiment.
From the results presented here we may also conclude that the dependence of χ and ν as given in the ABN-Set is not appropriate to describe the uncertainty which at present exists for the energy dependence of the fission spectrum. Recent measurements of NEILL [47] do not agree with the results of FABRY, GRUNDL, and MCELROY so that at present no definite conclusion can be drawn on the correct form of the fission spectrum.
A further uncertainty is caused by the fact that most fission spectrum measurements are performed for thermal fission in U235 or Pu239, whereas in a fast reactor the fissions are caused mainly by high energy neutrons. Most fission processes occur in U235 and Pu239 but a remarkable amount also in U238. For these fission processes there is considerable lack of detailed precise information on the energy dependence of the fission spectra.

III.3 Influence of different treatments of relatively thin reflecting zones

At the top and the bottom of the SUAK-assemblies there are reflecting zones which essentially consist of pure aluminum or iron. In these zones the cross sections are determined according to the usual ABN-procedure which for this case means practically total resonance self-shielding (σ_o=0). But the zones are only about 3 cm thick so that an asymptotic neutron energy distribution can never be obtained in these thin zones. Therefore the application of the σ_o-concept is rather doubtful. Most neutrons suffer at most one collision. Only those few neutrons which have energies corresponding to resonances with high peak values of the cross section suffer more than one collision within that thin layer of reflector material. Therefore the resonance structure of the neutron flux is not strongly marked and the assumption of total resonance self-shielding is not justified for these thin zones.
When reducing the influence of the resonance self-shielding by addition of the pseudo-material ANTIO it has been shown that the criticality of SUAK UH1B may increase by about 0.5%.

In one-dimensional transport calculations for the axial direction with transversal bucklings for the separated directions using the STRTR-transport cross section discussed in the next section and reflector cross sections for practically infinite dilution (σ_o = 1000 barn) an increase of k_{eff} has been obtained, compared to the usual results which correspond practically to total resonance self-shielding: Δk = +0.0065 UH1B (ABN-Set result), Δk = +0.0064 SUAK U1B (MØXTØT-Set result).

Table 3

Influence of resonance self-shielding for relatively thin reflecting zone

(by addition of the pseudo-material ANTI0)

Assembly	Group-set	Transport cross section	Δk
SUAK U1B	MØXTØT	STRTR	+0.0064
SUAK UH1B	MØXTØT	STRTR	+0.0061
SUAK UH1B	ABN	STRTR	+0.0065
SUAK U1B	MØXTØT	STR	+0.0095
SUAK UH1B	MØXTØT	STR	+0.0087
SUAK UH1B	ABN	STR	+0.0087

A preliminary result from heterogeneous calculations for SUAK UH1B with the ZERA-code resulted in an increase of k_{eff} by 0.49 (MØXTØT-Set result). For these calculations a strong absorber has be used at the outer boundary to simulate the vacuum boundary condition. Because of difficulties with the code in this special case which are due to the fact that for the pseudo-absorber material XY990 no transport cross section is provided no transversal buckling could be taken into account for the heterogeneity calculations.
Nevertheless it seems that both results indicate that taking into account properly the effect of the reflector zones present at the top and bottom yield an increase of the calculated criticality of about 0.5% which cannot be considered as to be small when comparing theory and experiment. It should be mentioned that with the previously used transport cross section STR the criticality increase observed

in the corresponding case is even larger, about +0.009 which is consistent with results discussed in the next section, where the influence of different types of transport cross sections is analysed having in mind that σ_o = 1000 barn is practically equivalent to infinite dilution, so that the differences between STRTR and STR practically disappear.
For natural uranium reflectors this effect is generally less pronounced than for iron-nickel- or aluminum-reflectors, because the f-factors for U238 in the important energy range are closer to unity than for the structural materials. For larger reactors the importance of this effect is reduced because of the lesser importance of the leakage process.

III.4 Influence of using different types of transport cross sections

In the diffusion calculations and up to the begin of 1970 also in the S_N-calculations the current-weighted transport cross sections (internal label STR) of the Russian ABN-set has been used. It is supposed that the flux weighted transport cross section (internal label STRTR) has to be used for reasons of consistency in the S_N-calculations. In this section all cross sections are calculated following the usual σ_o-procedures without using the pseudo-material ANTIO.
For SUAK U1B the use of STRTR instead of STR resulted in an increase of k_{eff} by 0.0030 for a one-dimensional transport calculation in the axial (z-) direction (MØXTØT-set-result). The leakage in the transversal direction is still determined with the transport cross section STR which corresponds to the diffusion calculations. This seems to be appropriate since the buckling for the separated space directions has been obtained by diffusion calculations. For the x- and y-directions a small decrease of criticality of -0.00016 has been obtained when using STRTR instead of STR. This is due to the fact that STRTR is not in all energy groups larger than STR in the MØXTØT-set, because the current weighted f-factors f_t have not been changed when going from the ABN-set to the SNEAK-set or other improved

versions of group constant sets, whereas for some isotopes all other f-factors which are flux-weighted have been redetermined and replaced.

The use of the STRTR-transport cross section instead of the STR-transport cross section used before causes an overall increase of k_{eff} of +0.0027 for SUAK U1B (MØXTØT-set-result). A similar result has been obtained for SUAK UH1B using the ABN-set: Δk_z = +0.00255, $\Delta k_x = \Delta k_y$ = +0.000375, Δk_{total} = +0.0033.

Table 4

Influence of the type of transport cross section (using STRTR instead of STR in S_N-calculations)

Assembly	Group-set	Pseudo-material with ANTIO in the reflecting zones	Δk
SUAK U1B	MØXTØT	no	+0.0027
SUAK UH1B	MØXTØT	no	+0.0026
SUAK UH1B	ABN	no	+0.0033
SUAK U1B	MØXTØT	yes	-0.0004
SUAK UH1B	MØXTØT	yes	+0.000002
SUAK UH1B	ABN	yes	+0.0010

III.5 Influence of the enrichment on the criticality of some SUAK-assemblies

With respect to the SUAK assemblies it seems worthwhile to mention that the atomic number densities used up to now are subject to some doubt. Especially the uranium enrichment appears to be probably too low because the patelets used in the experiments have been the same as those used in the SNEAK-facility whereas the enrichment reported in the literature for the SUAK assemblies is 19.86% compared to the enrichment reported e.g. for SNEAK 3A2 is 20.04%. Increasing the enrichment for the SUAK-assemblies to the value given for the SNEAK-facility leads to a criticality increase of +0.0055

for SUAK U1B and of +0.0038 for SUAK UH1B. Using recently revised data of WATTECAMPS [17] for the number densities of both assemblies causes an increase of the criticality of +0.0053 for SUAK U1B and of +0.0020 for SUAK UH1B.

III.6 Influence of the P1-approximation for the scattering on hydrogen

The influence of the anisotropic scattering on hydrogen in P1-approximation has been studied for SUAK UH1B using the consistent data of the ABN-set. At first a consistent value of k_{eff} has been determined for the different space directions x, y, z by onedimensional transport calculations. A value of $k_{eff} = 0.91498$ has been obtained with the corresponding bucklings: $Bx^2 = By^2 = 65.5541 \cdot 10^{-4}$ cm^{-2}, $Bz^2 = 55.6846 \cdot 10^{-4}$ cm^{-2}, B^2total $= 186.7928 \cdot 10^{-4}$ cm^{-2}. Taking into account the P1-approximation for the neutron scattering on hydrogen yields $k_{eff} = 0.91788$ with the corresponding bucklings: $Bx^2 = By^2 = 65.0221 \cdot 10^{-4}$ cm^{-2}, $Bz^2 = 55.2828 \cdot 10^{-4}$ cm^{-2}, B^2total $= 185.3265 \cdot 10^{-4}$ cm^{-2}. So the criticality difference caused by the influence of the P1-approximation for the scattering on hydrogen is $\Delta k = +0.0029$.

For a bare sphere of radius 19.64 which yields good agreement for k_{eff} determined by the successive onedimensional calcualtions in x, y, z direction using the transport approximation for the hydrogen scattering, the influence of the P1-approximation gives nearly the same result of $\Delta k = 0.0030$.

These corrections of 0.0029 respectively 0.0030 are smaller than the correction of 0.007 which has originally been assumed [11], [18] for the influence of the P1-scattering approximation on hydrogen.

On the other hand a fundamental mode calculation using the originally [11] determined total buckling of $205.33781 \cdot 10^{-4}$ cm^{-2} yields a $k_{eff} = 0.87913$ for the ABN-set which in turn gives a S_N-correction for k_{eff} of about $k = +0.036$ (ABN-set-result). This value is larger than the corresponding originally given value of 0.030 (SNEAK-set-result).

This fact shows that the S_N-correction depends to some extent on the set of group constants used. Therefore for major changes in the group constants the S_N-correction should be redetermined.

For SNEAK 3A2 the influence of the anisotropic scattering of hydrogen in P1-approximation is rather small as has been studied using the ABN-Set. For spherical geometry an increase of +0.0003 in k_{eff} has been obtained compared to the usual transport approximation for the scattering process (the transport cross section STR has been used). The same result has been determined by the addition of the corresponding corrections from one-dimensional axial and radial transport calculations (Δk_{ax} = +0.0001, Δk_{rad} = +0.0002) leading to a final k_{eff} of 1.0099 for the ABN-Set from the homogeneous transport calculations. For completeness it should be mentioned that the following consistent bucklings have been used: $B_{ax} = 8.2601 \cdot 10^{-4}$ cm^{-2}, $B^2_{rad} = 16.3408 \cdot 10^{-4}$ cm^{-2}.

III.B. COMMENTS ON INTEGRAL QUANTITIES

III.7 Material worth

The material worth measurements provide more detailed information on the neutron physics of the reactors to be studied than the criticality of the reactor systems. Although the principle of the method is very simple the interpretation of the measurements may be somewhat complicated.

The first difficulty is the absolute normalization because the experimental values are given relative to $\beta_{eff} \hat{=} 1\$$ and the theoretical value of the dollar is subject to some uncertainty as is shown for example for the assembly ZPR III-48 where PITTERLE [19] obtained 1% Δk = 942 ih whereas BROOMFIELD [20] reported a value of 1002 ih for 1% $\Delta k/k$.

To get rid of this difficulty one generally compares the material worth ratios between theory and experiment normalized most times to the U235 material worth.

The second difficulty is due to the fact that first order perturbation theory is in most cases not the adequate theoretical description for such measurements because it is valid essentially for an infinitely thin sample in a homogeneous core. Usually the samples in the actual measurements are plates of less than 1 cm thickness which are inserted in an environment which is heterogeneous because it is built by platelets containing different materials. Therefore a more appropriate theoretical model has to be applied than that of first order perturbation theory. In order to describe the interaction between the sample and the core appropriately one has to take into account the effect of flux depression in an absorbing material or flux peaking in a fissile material and the influence of resonance self-shielding which may be different for the sample and the surrounding core zone as has been pointed out by FISCHER [21].

The most severe limitations of FISCHER's method of treating the sample size effect are that it is not valid for very large samples and that it does not take into account the heterogeneous structure of the surrounding core.

OOSTERKAMP [22] constructed a special experimental device which enabled him to take into account in the calculations the influence of environmental effect. The following table shows a comparison of different theoretical results for material worth measurements in SNEAK-5C. The results have been taken from the work of OOSTERKAMP [22].

Table 5

Comparison of Different Results for Material Worths in SNEAK-5C

Isotope	Weight [g]	Position	P/O	F/O	O/Exp SNEAK-Set	O/Exp MOXTOT-Set
U238	60	1	0.84	0.80	1.16	0.95
	60	2	1.18	1.14	1.26	1.10
	5	1	0.54	0.61	0.80	0.72
	5	2	1.16	1.34	1.22	1.10
Pu239	5	1	0.90	0.93	1.09	1.04
	5	2	0.95	0.97	1.19	1.10
Pu240	3	1	0.90	0.81	1.44	0.91
	3	2	1.20	1.09	1.77	1.00
Fe_2O_3	3	1	-	1.24	0.55	0.55
	3	2	-	1.73	0.52	0.52
U235	3	1	1.00	1.00	1.00	-

P $\hat{=}$ First order perturbation theory

F $\hat{=}$ FISCHER's perturbation method of integral transport theory

O $\hat{=}$ OOSTERKAMP's improved version of the perturbation method of integral transport theory taking into account sample size and environmental effects

Exp $\hat{=}$ Experimental result

Position 1: Soft spectrum in the graphite region of the cell

Position 2: Harder spectrum in the fuel region of the cell

These results show that an insufficient theoretical treatment may cause errors of 10 - 20% or even more of the calculated material worth. The two last columns show that with the MOXTOT-Set the

agreement between theory and experiment is improved compared to the SNEAK-Set. Mostly the discrepancies are 10% or even less. Possible reasons for the two exceptions are discussed in [22].

The theoretical model of OOSTERKAMP which is well adopted to his special experimental device underlines the importance of environmental effects which have to be taken into accoung by the theory besides the effects of resonance self-shielding and the sample size of the probe.
The code seems to be superior to the codes RABBLE and RABID developed by KIER and others with respect to the computer time needed and to those of McGRATH and FOELL with respect to the treatment of resonance self-shielding as discussed by OOSTERKAMP [22].
When reporting on methods of calculation used to determine the material worth the results of KIEFHABER [23] should be mentioned . He studied the influence of group collapsing procedures on the calculated material worth. The results of the following table have been taken from [23].

Table 6 Results of First Order Perturbation Calculations with few Groups Normalized to the Corresponding 26-Group Results

Case	Weighting function of the few-group cross sections used for calculating			Number of few-groups	Central Reactivity worth for SNEAK-3A2 of							Neutron lifetime	β/l β=effective fraction of delayed neutrons
	ϕ	ϕ^+	$\delta\Sigma$		Al	C	Fe	Mo	Ni	U235	U238	l	
1	ϕ	ϕ	ϕ	11	0.949	0.999	0.989	0.999	0.935	1.007	1.012	0.973	1.026
2	$\phi^+\phi$	$\phi^+\phi$	$\phi^+\phi$	11	0.993	0.993	0.994	0.995	0.995	0.996	0.996	0.999	0.999
3	ϕ	ϕ	ϕ	5	0.728	0.621	0.593	0.969	0.898	1.054	0.950	0.945	1.067
4	ϕ^+	ϕ^+	ϕ^+	5	-1.112	0.183	3.778	1.404	3.754	0.757	-0.082	1.317	0.825
5	$\phi^+\phi$	$\phi^+\phi$	$\phi^+\phi$	5	0.976	0.979	0.992	0.984	0.986	0.985	0.987	0.995	0.989
6	ϕ	ϕ^+	$\phi^+\phi$	5	0.987	0.988	1.000	0.992	0.996	0.995	0.994	0.996	0.993

In case 1 and case 3 the usual flux weighting is used for the generation of the few-group-constants. Reducing the number of groups by about a factor of 2 leads to errors of up to 6.5% in calculated central material worth. A reduction by a factor of 5 causes errors of up to 40% especially for predominantly scattering materials. From case 6 can be seen that the use of the appropriate weighting procedures for the generation of the few group constants, which are now different according to their subsequent special use, leads to rather small errors of less than 1.85% for the calculated central material worth, even if the number of groups is reduced by a factor of 5.

Generally the group-constants of group sets with about 20-50 groups have been obtained by some sort of flux-weighting. No special attention has been given to the generation of group constants appropriate for adjoint flux- or perturbation-calculations. Therefore the results of the 26-group perturbation calculations may be subject to some systematic error. Especially for predominantly scattering materials it seems to be doubtful that one can definitely conclude from discrepancies between theory and experiment that there should be some error in the nuclear data and that these data have to be revised.
The results of PAGE and KUROSU [24] on the sodium void studies for ZPR III-48 confirmed this conclusion and give additional indications for possible sources of errors.

In the following table some results for the central material worths are given for two critical assemblies. The theoretical results have been determined by first order perturbation theory using the SNEAK-Set and the MOXTOT-Set. All values are normalized to U235. The experimental results for SNEAK 3A1 have been taken essentially from [9], those for ZPR III-48 from [19].

Table 7

Central Material Worths

Material	ASSEMBLY					
	SNEAK 3A1			ZPR III-48		
	Exp.	SNEAK-Set	MOXTOT-Set	Exp.	SNEAK-Set	MOXTOT-Set
U235	1.	1.	1.	1.	1.	1.
U238	-0.073 ±0.001	-0.0799	-0.0692	-0.074 ±0.002	-0.0780	-0.0678
Pu239	+1.47 ±0.04	+1.419	+1.377	+1.33 ±0.03	+1.336	+1.277
Pu240	-	-	-	+0.24 ±0.06	+0.065	+0.200
Na	-	-	-	-0.0018±0.0001	-0.0039	-0.0037
B10	-1.15 ±0.02	-1.219	-1.289	-1.12 ±0.02	-1.039	-1.061
Fe	-0.0062 ±0.0005	-0.0087	-0.0079	-0.0087±0.0004	-0.0103	-0.0095
Cr	-0.0050 ±0.0003	-0.0067	-0.0062	-0.0061±0.0003	-0.0085	-0.0085
Ni	-0.0106 ±0.0006	-0.0165	-0.0159	-0.0134±0.0003	-0.0166	-0.0162
Mo	-0.059 ±0.002	-0.069	-0.071	-0.052 ±0.001	-0.066	-0.065
C	+0.0085 ±0.0003	+0.0030	+0.0039	- -	-	-
Al	-0.00071±0.00008	-0.0027	-0.0021	-	-	-

From this table one may conclude:

a) The most obvious improvement has been obtained for the predicition of Pu240. This is due to improved nuclear data for Pu240 included in the MØXTØT-Set.

b) For U238 and Pu239 a better agreement between theory and experiment would be obtained if the calculated material worth of U235 would be reduced by about 5%. This would also result in a better agreement for the B10-worth in ZPR III-48.

c) For the predominantly absorbing material Mo it seems possible that the remaining discrepancy of 20-25% may be caused by sample size effects as can be seen in [21]. The discrepancy for the B10-worth in SNEAK-3A1 may be caused by the same effect.

d) For the structural materials Cr, Fe, Ni the environmental effect may be very important as can be seen in [22] probably together with sample size effects. The procedure used for the generation of group constants must also be considered as possible source of errors as mentioned just before.

e) For the predominantly scattering materials Na, C, Al the discrepancies between theory and experiment should not be taken too seriously because sample size effects play an important role (see [21]) and the procedure used for the generation of group-constants also may be responsible for some part of the discrepancies. The results presented by TILL [25] show the same tendency and therefore support the interpretation suggested above.

The final conclusion is that for most isotopes specific experiments have to be performed which can be compared with sufficient reliability with results of improved theoretical methods which take into account sample size and environmental effects. Furthermore, one has to study the influence of the procedure of the group constants generation using some hundred energy groups for the basic calculations.

In the following we will discuss the influence of the model of calculation applied for the determination of the central material worths. Three

items have been studied which are often encountered in practical problems: a) the influence of the number of energy groups, b) the influence of the number of mesh points, c) the influence of the geometrical model used, i.e. one- or two-dimensional geometry. The results are shown in the following table.

The influence of the number of energy groups was discussed before extensively. Here one should mention only that usual flux weighting has been adopted for the collapsing procedure and that the original 26-group weighting flux has been obtained by a onedimensional calculation for a spherical model of the assembly.

The influence of the number of mesh points on the central material worths is far less severe than the number of energy groups. The largest differences can be observed for the predominantly scattering materials C, O, and Mg. But even for oxygen showing the maximum deviation of about 15% upon reducing the number of mesh point by a factor of 4 the deviation must be considered as small compared to the fact that a reduction of the number of energy groups from 26 to 4 leads to a change of sign in the material worth for the same material.

As could be expected a onedimensional model of this assembly with a large practically uniform core-zone provides sufficient accuracy for the determination of the central material worth. With respect to the present range of uncertainty all differences obtained between the one- and twodimensional model can be considered as negligible.

Table 8 Comparison of the results of perturbation calculations for SNEAK 3A2

Quantity	Model of Calculation				
	2-dim.cyl. 26 energy groups	2-dim.cyl. 11 energy groups	2-dim.cyl. 4 energy groups	2-dim.cyl. 4 energy groups	1-dim.spherical 26 energy groups
Central Material Worth for 10^{20} atoms of	1600 mesh points	1600 mesh points	1600 mesh points	400 mesh points	
Al	-0.204 /-9	-0.198 /-9	-0.235 /-9	-0.236 /-9	-0.208 /-9
B^{10}	-0.221 /-6	-0.217 /-6	-0.219 /-6	-0.221 /-6	-0.221 /-6
C	0.486 /-9	0.489 /-9	0.195 /-9	0.203 /-9	0.474 /-9
Cr	-0.821 /-9	-0.849 /-9	-0.577 /-9	-0.581 /-9	-0.822 /-9
Fe	-0.109 /-8	-0.109 /-8	-0.918 /-9	-0.926 /-9	-0.109 /-8
H	0.144 /-7	0.148 /-7	0.122 /-7	0.125 /-7	0.142 /-7
Mg	0.637 /-10	0.787 /-10	0.129 /-9	0.136 /-9	0.567 /-10
Mo	-0.115 /-7	-0.116 /-7	-0.113 /-7	-0.114 /-7	-0.115 /-7
Ni	-0.222 /-8	-0.225 /-8	-0.209 /-8	-0.211 /-8	-0.222 /-8
Ø	+0.427 /-9	+0.438 /-9	-0.370 /-10	-0.316 /-10	+0.417 /-9
Pu239	0.166 /-6	0.166 /-6	0.168 /-6	0.170 /-6	0.167 /-6
U235	0.121 /-6	0.120 /-6	0.123 /-6	0.125 /-6	0.122 /-6
U235	-0.851 /-8	-0.863 /-8	-0.795 /-8	-0.801 /-8	-0.848 /-8
Neutron lifetime	0.3897/-6	0.3847/-6	0.3877/-6	0.3884/-6	0.3893/-6

III.8. Decay constant and neutron lifetime

The discrepancies between the experimental and theoretical results for the neutron decay constant α and the neutron lifetime l may in part be due to the same difficulties as those encountered in the chapter on material worth. Because of the relation $\alpha=\beta_{eff}/l$ there is the same problem of the determination of β_{eff} as mentioned for the normalization of the material worth measurements (see also e.g. LITTLE and HARDIE [26]). Recently the absolute delayed-neutron yield for U238 has been determined by MASTERS et al. [27] to be about 14% larger than the generally used value of KEEPIN [28]. The uncertainty quoted by MASTERS, however, is rather large, about 30% so that KEEPIN's result - with a quoted error of about 7% - is still well within the error limits of MASTER's result.

It seems worthwhile to note, that MASTER's results show a remarkable dependence of the total delayed-neutron yield on the incident neutron energy in the range 3-14 MeV. Furthermore, this dependence is in contradiction to earlier results of MAKSIUTENKO taken from [28].

From the procedure of calculation the neutron lifetime can be considered as a material worth too. Therefore, the same doubts on the accuracy and reliability of the method of calculation are justified as for the material worth. From the two last columns of table 6 (see also [29]) it can be seen, especially from cases 1 and 3, that a reduction of the number of energy groups using the usual collapsing procedure leads to an underprediction of the neutron lifetime of 2.7% respectively 5.5% going from 26 groups to 11 respectively 5 groups. This error is mainly due to the insufficient prediction of the low-energy neutron importance.

In summary one may conclude that

a) there is some uncertainty in the total delayed-neutron yield for U238 and the dependence of this value on the incident neutron energy

b) there is some doubt if the presently used sets of flux weighted group constants with about 50 or less energy groups gives sufficiently accurate and reliable results for the neutron lifetime.

c) In addition to these two effects other effects e.g. the influence of heterogeneity (see [30]) must probably be taken into account for the appropriate theoretical determination of the prompt neutron decay constant and the neutron lifetime.

III.9. Doppler effect

In 1966 the prediction of the Doppler effect for U238 was subject to an uncertainty of about ±30% as can be seen from the intercomparison calculations for ZPR III-48 [3]. For ZPR VI-5 TILL [25] reported in 1969 an underestimate of the U238-Doppler effect by about 25% whereas the reactivity worth of a fuel plate for the same assembly was overestimated by about 10% in the calculations. An underestimate of 20-30% for the U238 Doppler effect was reported also by HÄGGBLOM and TIREN [31]. They obtained an overprediction by factors of 2 to 4 for the U235- and Pu239-Doppler effects. At Karlsruhe the situation seems to be somewhat more satisfactory: For the U238 Doppler effect in SNEAK-3A2 the deviation between theory and experiment amounts to 5% or less as is shown in [32]. For the calculations the method of FISCHER [33] has been used. The statistical resonance parameters were taken from SCHMIDT [34]. For U238 the resolved resonance parameters of GARG et al. [35] have been used. The samples of UO_2 were of different enrichments: 0.4%, 15% and 25% and for all of them the maximum deviation was about 5% or less. Even for samples of PuO_2 the deviations were generally less than 20% in case the resonance parameters of PITTERLE [36] were used. With the earlier resonance parameters of SCHMIDT [34] a remarkable disagreement between theory and experiment was observed. Therefore these measurements strongly favour the resonance parameters of PITTERLE and thus were a strong indication

of higher α-values of Pu239 in the keV-region. A detailed description of the measurements and their analysis has been presented by FISCHER [37] who indicated that an uncertainty of at most 15% in the calculated Doppler effect for these plutonium sample measurement may be caused by the overlap effect between U238 and Pu239 resonances. In [37] it is also shown that the Doppler effect measurements for a $U_{nat}O_2$-sample in ZPR VI-4Z can also be predicted with a 10% deviation. Further information on SNEAK-3-measurements [38] confirmed the conclusion that at Karlsruhe the fuel Doppler effect can be predicted with an accuracy of about 10%.

It seems that the experimental set-up used for the Doppler experiments and the theoretical methods used for their interpretation correspond rather well to each other. The fact that the measurements and calculations are refined enough and well suited to each other must be considered as the reason for the remarkably good agreement in the determination of the Doppler effect observed at Karlsruhe.

III.10. Reaction rate measurements and cell traverses
(Influence of the model of calculation)

In earlier times a lot of reaction rate measurements especially fission ratio measurements have been performed using fission chambers as detectors. These measurements are now considered as not very precise and reliable because they are subject to systematic deviations of the order of 5 to 10% [39] which are due to spectrum distortions caused by the chamber. BÖHME and SEUFERT [40] have shown that for SNEAK 3A2 the fission ratio σ_{f8}/σ_{f5} obtained by chamber measurements is about 8% lower than that obtained using foil measurements. Therefore, one has to be cautious if there is disagreement between theory and experiment for older reaction rate measurements.

At present one is able (see [25] [41]) to measure reaction rates using different independent experimental techniques, e.g. radiochemistry, foil measurements, track detectors etc., in order to have a cross check for the experimental results, so that undetected systematic errors become rather unprobable. Unfortunately some of the experiments and/or experimental techniques are not described in full detail. Therefore, it is sometimes difficult to get an impression of the correctness and reliability of these experiments and to make

use of them for the check of differential nuclear data by integral measurements.

At Karlsruhe not all of the new independent techniques are fully developed. Some experience has been gained with respect to foil measurements [40]. It has been shown by recent calculations discussed in the following that in these experiments the normal cell is disturbed to some extent by the introduction of the foils. This perturbation cannot be neglected when comparing theory and experiment. A reduction of the foil thickness would reduce the perturbation and at the same time some doubts on the correctness of the determination of the U238 capture rate [42] would no longer be important. For the SNEAK-3A2 experiments [40] in the unbunched cell six foils (three of depleted and three of 20% enriched uranium, each 0.01 cm thick) have been placed into the somewhat modified fuel platelet of 20% enriched uranium which normally has a thickness of 0.314 cm.

The influence of the introduction of the foils has been studied theoretically using the ZERA-code of WINTZER [30]. In the following table the essential results are given:

Table 9

ZERA-calculations for the unbunched SNEAK-3A2-cell

	k_{eff}	$\frac{\sigma_f U238}{\sigma_f U235}$ 1)	$\frac{\sigma_c U238}{\sigma_f U235}$ 1)
case I	1.00197	0.02757	0.1207
case II	0.9748	0.0262	0.1184
case IIa	1.0022	0.02565	0.1186
case III	1.0681	0.0280	0.1190
case IV	1.0304	0.02647	0.1177

1) these values are valid for the fuel platelet only

case I: normal cell without any perturbation. The atomic number densities have been obtained assuming the edge length of the platelets to be 5.44 cm. They include the homogenized stainless steel of the subassembly wall.

case II: as in case I but 3 pairs of foils introduced into the modified fuel platelet. The foils of 0.01 cm are assumed to extent over the whole 5.44×5.44 cm^2 area with their correct surface mass loading of about 0.18 $/\bar{}g/cm^2\_/$.

case IIa: as in case II but the buckling has been reduced by 10% to obtain about the same value for the criticality as in case I.

case III: normal cell without perturbation. The atomic number densities present on the central axis of the cell have been used. Edgelength of the platelets 5.068 cm. The stainless steel of the subassembly wall has not been taken into account.

case IV: as in case III but 3 pairs of foils have been introduced into the modified fuel platelet in the same manner as in case II.

From the results presented in this table the following conclusions can be drawn:

a) Introducing the 3 pairs of foils into the fuel platelet causes a severe perturbation of the normal cell and leads to a remarkable reduction of the ratio σ_{f8}/σ_{f5} and to a less pronounced reduction of the ratio σ_{c8}/σ_{f5}. The main reason is the reduction of the average enrichment of the modified fuel platelet (including the foils)

b) The observed reductions of the reaction rate ratios are nearly independent of the models adopted for the calculations, i.e. the procedure used for the determination of the atomic number densities.
This fact is very favourable because, according to the experimental

set-up, it must be expected that these foil measurement in SNEAK-3A2 mainly describe the situation present on the central axis of the cell so that a homogenization of the platelets and tube walls over the whole area of the element tubes may be considered as a somewhat doubtful model for the description of these experiments.

c) If one assumes that the perturbation within the cell leads also to a distortion of the flux distribution in the neighbourhood, the leakage will be changed. This has been simulated in case IIa where the buckling has been adjusted in such a way as to give about the same criticality as has been obtained for the normal undisturbed cell. This leads to a further reduction of the ratio σ_{f8}/σ_{f5} whereas the ratio σ_{c8}/σ_{f5} remains nearly unchange.

Although it has been shown that the reaction rate ratios are only weakly dependent on the calculational model adopted for the determination of the atomic number densities, i.e. concentrations present on the central axis of the cell or concentrations obtained by homogenization including the subassembly wall, it is discussed below that the reaction rate traverses within the fuel platelet show an appreciable influence on the calculational model. This holds especially for the fission rate in U235 which is very sensitive because it is composed of two components of opposite tendency: the high energy component which is peaked and the low energy component which is depressed in the fuel platelet.

A comparison of the two cases mentioned above (case I and case III of the preceding table) is shown in Fig. 4 where it becomes apparent that the depression of the U235 fission rate in the fuel platelet is considerably influenced by the calculational model.

For the case where the high atomic number densities of the cell axis are used it may be argued that the spectrum is not representative for the real situation because

a) the surrounding steel wall has been neglected so that the scattering probabilities and the resonance self-shielding are modified,

b) the higher concentrations lead to larger transport cross sections so that the leakage is reduced ,

c) the resulting larger value for criticality (1.068 instead of 1.002) may cause a shift of the neutron spectrum.

Since there is no calculational model, which allows to take into account appropriately all these effects simultaneously a third calculational model, suggested by WINTZER, has been applied to get some idea of the influence of the drawbacks mentioned above. Here the cell has been modified in such a manner that the correct cell averaged composition is maintained.

The thickness of the fuel-platelet is 0.314 cm as it is in reality. The atomic number density is that present at the cell axis as in the case studied before. In order to obtain the correct cell averaged composition, the thickness of the whole cell has to be increased from the original value of 1.256 cm to the modified value of 1.447 cm. This leads to a modified thickness of 0.3777 cm for the three remaining platelets of the modified cell. The steel of the subassembly wall has been homogenized into these three remaining platelets (SS+CH_2, Al 25%, Al_2O_3) and the atomic number densities for the materials of these platelets has been determined in such a way, that the cell averaged composition is correct. This is indicated by the fact, that the criticality value of 1.007 is in approximate agreement with that for case I which is equal to 1.002.

For this model the dashed curves in Fig. 5 have been determined, which are compared with curves obtained for case I corresponding to a complete homogenization over the area of 5.44×5.44 cm^2 (low uranium concentration). It can be seen from Fig. 5 that the change in the depression of the U235 fission traverse in the fuel platelet is less pronounced than in the preceding Fig. 4. On the other hand in Fig. 5 the change in the peaking of the U238 fission traverse is more pronounced than in the preceding Fig. 4. It is supposed that this effect is caused by the fact that the concentrations mainly of oxygen and aluminium in the Al_2O_3- respectively Al25% platelet adjacent to the fuel platelet are somewhat lower in the case of the modified cell than in case I. Therefore, because of the reduced

density and poorer reflector properties respectively increased transparency obtained for the adjacent platelets it seems plausible that the removal of high energy neutrons is slightly more pronounced in the outer parts of the fuel platelet than in case I. This fact would be more evident if the two curves for fission in U238 in Fig. 5 would have been normalized at the center of the fuel platelet and not - as is actually done - at the outside of the fuel platelet.

An increased removal of high energy neutrons is also indicated by the fission ratio σ_{f8}/σ_{f5} which is equal to 0.02727 for the modified cell compared to 0.02757 for case I. (σ_{c8}/σ_{f5} = 0.01201 for the modified cell and =0.1207 for case I.)

The change in the depression of the U238 capture traverse in the fuel platelet is about the same in Fig. 4 and Fig. 5. This means that compared to the case of complete homogenization (case I) the two cases of high uranium atomic number densities in the fuel platelet, namely the calculation with the concentrations present in the cell axis and the calculation for the modified cell lead to about the same curve for the U238 capture rate in the normal fuel platelet.

III.11. Reaction rate traverses within the cell

(Comparison of theory and experiment)

BÖHME and SEUFERT measured the reaction rate traverses within the cell using foils of about 0.01 cm thickness. Two uranium foils were placed together one of about 20% the other of 0.44% enrichment. In Fig. 6a, 6b, 6c the calculated reaction rate traverses for an idealized case are shown. Here the concentration of uranium both U235 and U238 in the non-fuel platelets has been assumed to be smaller by a factor of 1000 than that present in the fuel platelet. This is a good approximation for the unperturbed cell. In reality the pair of foils present in the non-fuel-platelets lead to appreciably higher uranium concentrations when averaged over the

platelets in which they are inserted. The form of the cell traverses are nearly independent of the uranium concentrations in the non-fuel platelets used in these two cases except for the capture rate in U238, where a considerable reduction in the non-fuel platelets is observed for the second case compared to the first case as is shown in Fig. 7.

Fig. 6c shows that the average reaction rate for fission in U235 in each platelet can be determined rather accurately even in the case when in the calculation each platelet is taken as one region without any further subdivision. For capture and fission in U238 shown in Fig. 6a and Fig. 6b the agreement for the average reaction rate in the platelets determined with 4 and 14 subregions per cell respectively is even better than that shown in Fig. 6c for fission in U235.

In the next two cases described below we have taken into account the real experimental situation in more detail. Especially we really considered the case where a foil of polyethylene was placed into the partially empty stainless steel platelet.

A) In the first case we have averaged the uranium foils of 0.1mm thickness and 25.4 mm diameter over the whole lattice area (5.44×5.44 mm^2) keeping the thickness of 0.1 mm and the total amount of uranium constant thus obtaining reduced uranium concentrations compared to reality.

B) In the second case we assumed that the foils with the real thickness and surface mass loading would extend over the whole lattice area, thus obtaining uranium concentrations which correspond to those valid for the central axis of the cell. But thereby the total amount of uranium in the foils has been overestimated by a factor of 5.84. Because the

ZERA-code can handle only one-dimensional geometry it is not possible to take into account the experimental situation in a more sophsiticated model. *)

A comparison of the calculated results with the experimental results of BÖHME and SEUFERT is given in Figures 8a, 8b, 8c, 9. As has been known before, there is no good agrement for the U235 fission rate. (a different normalization for example in the center of fuel platelet would not remove the observed discrepancies). For the U238 fission rate there is a rather good agreement in the fuel platelet between theory and experiment. The discrepancy in the Al-platelet may be caused by the fact that for the calculations the concentrations for the normal SNEAK-Al-platelets have been used whereas for the experiments special Al-platelets have been fabricated for which the concentrations are not given in [40]. In the SS+CH_2-platelet numerical difficulties may partially be responsible for the discrepant behaviour of the calculated and measured U238 fission rate and probably also for the U235 fission rate. For both fission rates there are only negligible differences in the space dependence within the cell between the cases A) and B).

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*) Even for the cases considered here we encountered some numerical deficiencies:

a) the approximation of the E_3-function by a sum of exponential functions is only valid with good accuracy for optical thickness between 0.002 and 2.0 so that for optically thin zones especially for practically empty zones the reliability of the results becomes questionable

b) if there is a nearly empty zone within the cell one cannot take into account a universal buckling for all zones of the cell because the leakage determined with the present version of the code would no longer be meaningful. To avoid this difficulty we used $B^2=0$ for this special nearly empty zone, using the usual value of B^2 for the other zones.

For the U238 capture rate the situation is somewhat more complicated. In the measurements only the depleted uranium foils have been used for the determination of the capture rate, the enriched uranium foils have been disregarded.

In Fig. 8a and Fig. 9 the position of the foils is always such that the depleted uranium foil is at the right hand side of the enriched uranium foil for the pair of foils which was always inserted into the platelets. In the calculations as well as in the experiments the foils were distributed over two adjacent cells in order to keep the additional uranium content in the cell or in other words the perturbation of the normal cell introduced by the foils as low as possible.

The differences in the U238 capture rate between the two neighbouring foils in the pair of foils is considerable as can be seen from Fig. 8a and Fig. 9 where we have tried to indicate the position of the foils. It is important if there is another foil of uranium between the most important source region for low energy neutrons and the special uranium foil considered. Comparing Fig. 8a and Fig. 9 it is obvious that the experimental results are within the uncertainty range of the theoretical results. This is caused by the fact that in the calculations the real experimental situation cannot be taken into account appropriately but insufficient approximate models have been used instead.
This calls

α) for a more simple experimental arrangement for which a more unique model for the calculations can be provided and/or

β) for a more sophisticated heterogeneity code which is able to describe adequately the rather complicated geometric configuration encountered in the experiment.

From the present study of the fine structure of reaction rate traverses in the unit cell of SNEAK 3A2 the following conclusions can be drawn

I) Some numerical deficiencies in the ZERA-code should be removed especially those concerning zones of small optical thickness and the output for the neutron fluxes which should be made consistent with the corresponding output for the reaction rates.

II) One should try to simplify the experimental arrangement so that a relatively simple, adequate model of this arrangement can be used with sufficient accuracy for the calculations.

III) If item II cannot be realized only a new, more elaborate code would provide the necessary mean for a reliable evaluation of the fine structure traverses.

III.12. Reaction rate traverses through core and blanket

As an example of reaction rate traverses we will consider here the measurements of BÖHME and SEUFERT [40] in SNEAK 3A2. They measured the traverses with foils and corrected their results for the heterogeneity effect present in the normal cell using results determined also by specific experiments. For the comparison of calculation and experiment all curves in the figures 10-14 are normalized to unity at the core center in order to get rid of deviations observed when comparing theoretical and experimental results for the central reaction rates.

In Fig. 10 the results presented in the original work are shown (SNEAK-set results). The deviations are about 3% in the core region and up to about 25% in the blanket region. It should be mentioned that the discontinuity due to the different resonance self-shielding in the core and blanket region which is rather pronounced for the U238 capture, is not shown in the original work for this figure. In Fig. 11 the results of a recent recalculation with the MOXTOT-set are shown. For the calculations heterogeneity corrected cross sections for the core zone are used.

Here S_6-transport calculations are applied whereas for Fig. 10 (i.e. the original work) diffusion calculations have been used.

The agreement between theory and experiment is improved compared to the previous results. This is mainly caused by the used of the S_6-calculation and the application of the improved nuclear data included in the MOXTOT-Set.

It has been shown that at the core-blanket boundary heterogeneity effects occur which are caused by the platelet structure of the core zone and by the exchange of neutrons between the core and the blanket region which is essentially composed of depleted uranium metal. When takinginto account these effects especially the pronounced change of resonance self-shielding for U238 capture one obtains the results presented in Fig. 12. It can be seen that the maximum deviations in the core region are about 4% and generally less than about 10% in the blanket region. Especially in the blanket region a considerable reduction of the discrepancies shown in the original work between theory and experiment has been obtained. In addition the discontinuity at the core-blanket interface for the U238 capture essentially disappeared.

The improved agreement observed for the outer blanket region is partially due to the fact that the influence of the reflecting material present outside the blanket has been taken into account. It can be seen from Fig. 11 and Fig. 12 that precise measurements in the outer blanket region would be sensitive to the influence of the reflector. The differences between the theoretical results for a weak and a somewhat stronger reflector can be detected within the outer 5 cm of the blanket as is shown in Fig. 11 and Fig. 12.

The still remaining discrepancies between theory and experiment for the reaction rate traverses are about twice as large as the experimental uncertainty. Especially for the fission traverses in the blanket the experimental accuracy and reliability seems to be not sufficient to draw conclusion from the discrepancies observed.

The discrepancies apparent at the core-blanket-interface may be caused by an inadequate prediction of the neutron energy distribution in this transition region .
The discrepancies of the traverses in the core region could be reduced if the core would become more transparent for the neutrons e.g. by a hardening of the neutron spectrum or by a reduction of the transport cross section especially below about 150 keV. This energy range is most important for the U238 capture- and U235 fission rate which are somewhat more discrepant than the U238 fission rate in the core region.
The discrepancies for the U238 capture rate in the blanket show a systematic tendency contrary to the U235 and U238 fission rates where no systematic deviations can be observed. This supports the statement of the experimentalists that the measurement of the U238 capture rate in the blanket could be considered as reliable. Possible improvements could be obtained by increasing the transparency of the core- and blanket composition by spectrum hardening or reduction of the transport cross section. The easiest but not necessarily most probable or most correct way, however, would be to reduce slightly the removal cross section of the blanket material in the energy range of about 1-100 keV, which would also improve the agreement for U238 capture and U235 fission traverses in the core region. A reduction of the removal cross section of the blanket composition is practically equivalent to a reduction of the capture cross section of U238. At first glance a change in this direction seems to be not very probable because the capture cross sections of U238 used in the MOXTOT-set are already rather low and and the resulting ratio $\sigma_c(U238)/\sigma_f(U235)$ is generally underpredicted However, one has to realize that in the blanket which is essentially built of depleted uranium the U238 resonances are strongly self-shielded. Therefore, a reduction of the macroscopic effective capture cross section could be obtained by a reduction of the self-shielding factors, keeping the infinite dilute values constant. This fact shows that in the future the f-factors of U238 should be reconsidered.

The results of fission chamber traverses for U235 fissions are compared with the theoretical results in Fig. 13 and Fig. 14. Fig. 13 represents the original results of BÖHME and SEUFERT (SNEAK-set results), whereas Fig. 14 shows the most recent, best available theoretical results obtained with the MOXTOT-set. Here especially in the outer blanket region rather large deviations between theory and experiment can be observed which cannot be explained by the influence of the reflector. Because such deviations are not apparent for the foil measurements of the U235 fission traverse it can be concluded that the supposition expressed in [32] seems to be true, that the results of the chamber traverses have to be considered as doubtful because of streaming effects present in the channel used for the measurements Thesestreaming effects tend to increase the measured reaction rate in the outer parts of the assembly so that the ratio of theory to experiment is reduced compared to that which would correspond to measurements which are free of streaming effects. In the subsequent experiments the experimental set-up will be modified in order to reduce the influence of streaming effects for the chamber measurements of traverses.

Heterogenity at the core-blanket interface

It can be seen from Fig. 10 and Fig. 11 that there is a step in the U238 capture and U235 fission rate at the core-blanket interface for the usual calculations. This is due to the fact that the resonance selfshielding factors are different in the core- and blanket region respectively because of the different material compositions and the resulting different background cross section σ_o in both regions. In reality of course there is no stepwise but a continuous transition for the reaction rates when crossing the core-blanket interface. Work is underway [48] to take into account this effect of space-dependent resonance self-shielding factors near interfaces between different compositions under the assumption of plane geometry and homogeneous mixtures in the different space regions.

Even if this code will be available it can probably not be applied in a meaningful way for SNEAK 3A2 because the main effects occur within the range of one mean free path distance from the boundary so that the assumption of homogeneity of the core composition would be a too crude approximation. Therefore, the heterogeneity code ZERA has been applied to get an idea of the influence of heterogeneity at the core-blanket interface. Since the code could only handle the periodic boundary condition for plane geometry the same boundary condition had to be applied in the corresponding S_6-calculations performed to study the influence of heterogeneity and using transport theory in both cases (using the transport cross section labelled STRTR).

In the ZERA-calculation 10.048 cm (8 cells) of the core region, the half-platelet of stainless steel (o.157 cm) present at the interface and 6 cm of the blanket region have been considered. In the S_6-calculation 10.048 of the homogenized core-region and 6.157 cm of the blanket region have been taken into account. The half-platelet of stainless steel at the interface is replaced by blanket material in the calculational model as is usually done in the diffusion- and S_N-calculations for determining the reaction rate traverses.

In Fig. 15 and Fig. 16 the results for the traverses obtained by the ZERA- and S_6-calculations are compared. The averages in the platelets are given and the fine-structure within the platelets is indicated. (In the S_6-calculations no platelets have been considered but a homogenized core composition.)

For the capture rate of U238 it can be seen from Fig. 15 that the ZERA-results in corresponding platelets are lower than the S_6-results in the outer part of the core compared to the inner part of the core. Within the first few tenths of a millimeter in the blanket the ZERA-results are considerably larger than the S_6-results. If numerical effects can be disregarded this can be considered as an effect of the space dependence of the resonance self-shielding factors. It can be seen from Fig. 15 and in more detail from Fig. 17 that the asymptotic behaviour is approached very soon within the

blanket. Furthermore Fig. 15 gives an idea of the pronounced fine structure of the U238 capture rate due to the effect of heterogeneity of the platelet-arrangement.

For the U235 and U238 fission rate shown in Fig. 16 this fine structure of the reaction rate is far less marked than for the U238 capture rate. For the U235 fission rate there is a slight decrease of the ratio ZERA-result/S_6-result with increasing distance from the core center.

The U238 fission rate shows a slight increase of the ratio ZERA-result/S_6-result with increasing distance from the core center up to that distance where the last Al_2O_3-platelet is placed. It could be argued that the strong removal of high energy neutrons caused by this platelet or the different energy dependence of the transport cross section of Al_2O_3 compared to the average core composition are responsible for the behaviour. But it seems to be more probable that numerical effects are responsible for this effect. The application of the S_6-approximation at the boundary between rather different material compositions and between regions of different neutron source density may be doubtful especially if a very small mesh is used as has been done in our case.

Possible influence of heterogeneity effects on reaction rate traverses in the blanket

The presence of the 20% enriched uranium foils in the blanket will lead to local peaks in the fission distribution so that this distribution deviates from the distribution which is normally present in the blanket without foils. This means that the environment is disturbed compared to the normal situation similar to the case where the foils were placed within the fuel platelet. Thus the measurements may not show correctly the normal traverses but some modified traverses. It is supposed that the deviations are most pronounced for the fission in U238 because this reaction rate is most sensitive to the additional fission neutrons produced by fissions in the 20% enriched uranium foil. The fission in U235 probably is also influenced to a certain amount. The U238 capture rate is supposed to be rather insensitive to this effect, but detailed studies will be necessary to obtain quantitative results.

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APPENDIX

V. SIGNIFICANCE OF ADJUSTMENT PROCEDURES FOR GROUP CONSTANTS

At the International Conference on Fast Reactor Physics held 1969 in London many reports on nuclear data adjustment were presented. In BAKER's survey of this conference [49] one reads: "In the UK and several other countries it is now realized that systematic adjustment of the best evaluated data by a least-squares fitting process will be necessary to obtain adequate agreement for integral measurements and adequate accuracy on the time scale required for reactor design".

It seems to us that the last part of this statement is most important namely the time scale for the design of the prototype reactor. The uncertainties in the physics prediction for such a reactor which existed in the past and partially continue to exist up to now have been and probably are still rather large from the point of view of the designer of such a reactor who wants to have more precise specifications for example for the fuel enrichment or the expected breeding gain or the reactivity change during burn up. These demands present a rather strong incentive to develop adjustment procedures. Their main significance has to be considered in connection with the rather tight time scale of some nations building prototype reactors.

On the other hand the still existing discrepancies between predicition and measurement for integral quantities is a challenge for the theoretical and experimental physicists to find out the reason for the disagreement and to improve the theoretical and experimental methods. For the theory this means to examine and if necessary to improve

(a) the basic nuclear data,
(b) the methods and codes for the generation of group constants,
(c) the methods and codes used for the calculation of integral quantities.

At the London Conference there were some doubts whether such a data adjustment is a meaningful procedure. This can be also found in BAKER's survey [49]:"The big question that hangs over data adjustment

that was aired at the panel discussion was this: Do we really get more accurate data that will give better predictions of all kinds or are they merely fitting parameters in an interpolation procedure?" The panel did not come to a final conclusion and unfortunately BAKER also did not try to give an at least tentative answer to that important question in his survey [49].

DRAGT [50] considers the problem of data adjustment from a more mathematical and statistical point of view. One of his conclusions which is important for our present discussion is the following: "It is often not true that adjustment procedures improved values for the differential data".
Therefore, the main advantage and importance of the adjustment procedures in our opinion consists in the fact that because of the improved agreement observed between theory and experiment for integral quantities of fast assemblies when adjusted data are used one hopefully can expect that the prediction of similar quantities for fast power reactors will be more reliable than with unadjusted data provided that for the calculation of the power reactors the same methods are and can be applied which have been used for the calculation of the criticals forming the basis for the adjustment. But one should always have in mind that this does not mean that the adjusted data are really improved or that the methods of calculation and models employed are correct or provide sufficient accuracy.

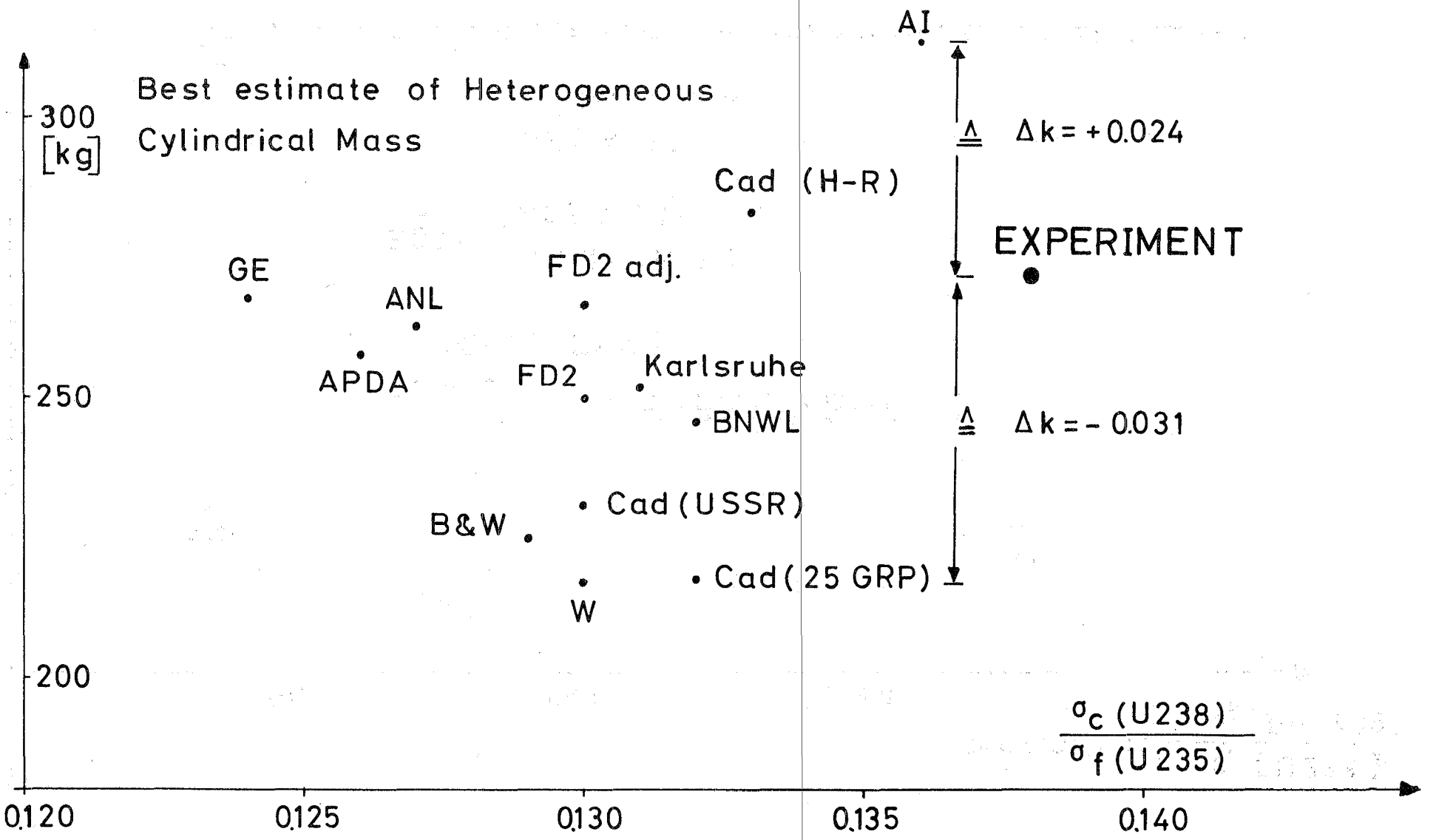


Fig. 1 Results of Intercomparison Calculations for ZPR III -48 in 1966

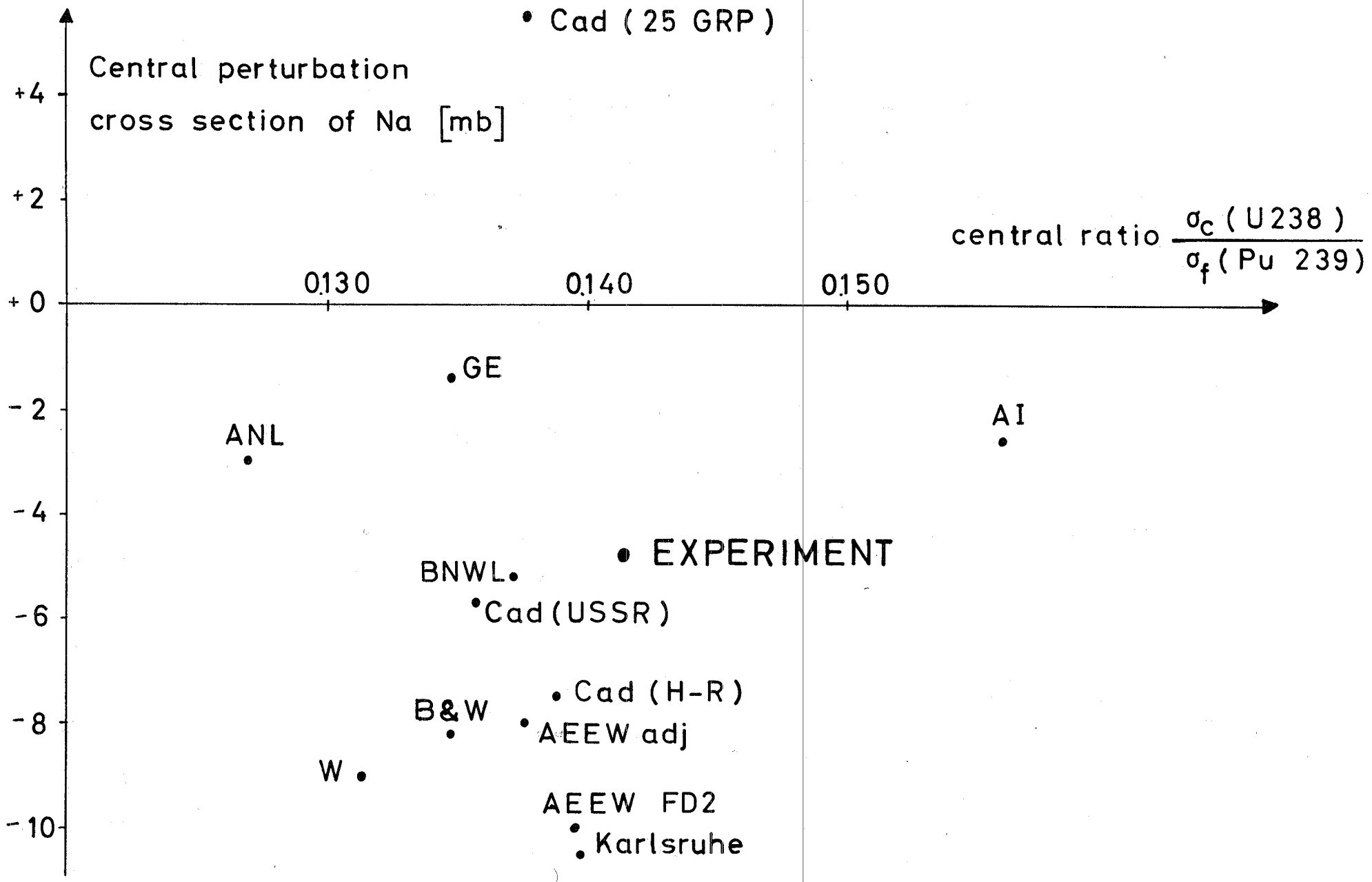


Fig. 2 Results of the Jntercomparison calculations for ZPR III-48

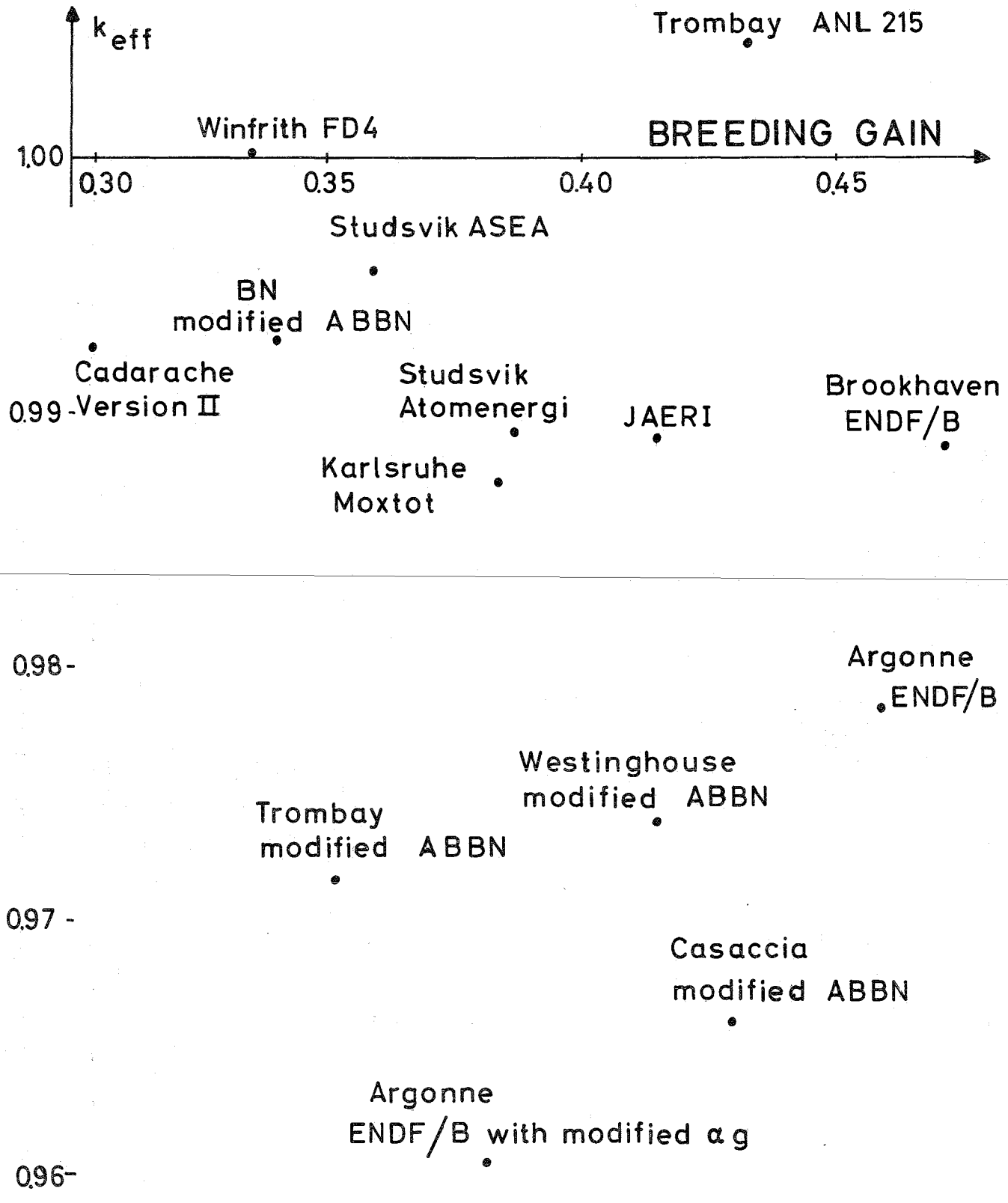


Fig.3 Results of standard reactor calculations in 1969. keff for identical reactors
Breeding gain for critical reactors

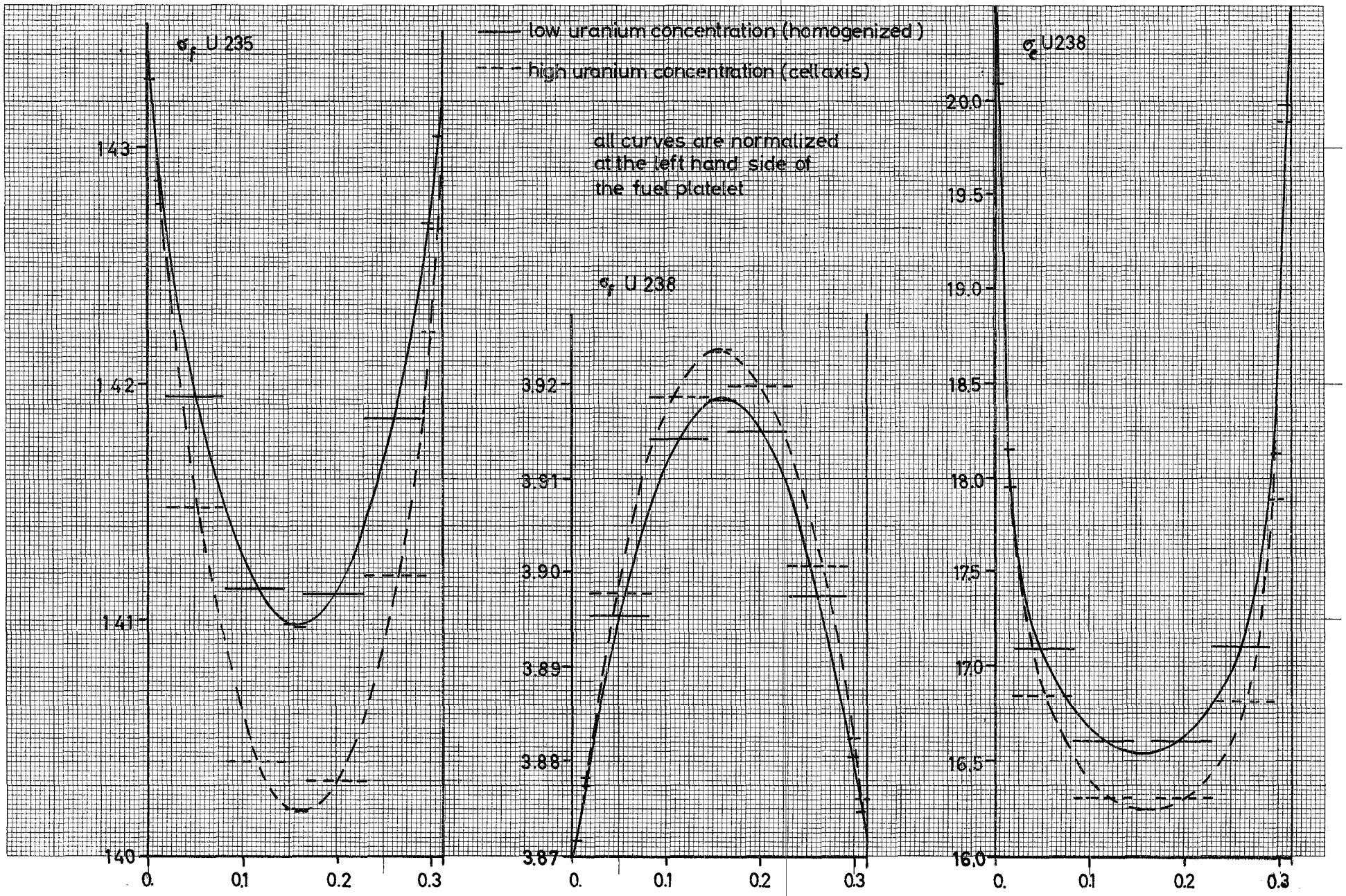


Fig. 4. Comparison of reaction rate traverses in the normal fuel platelet

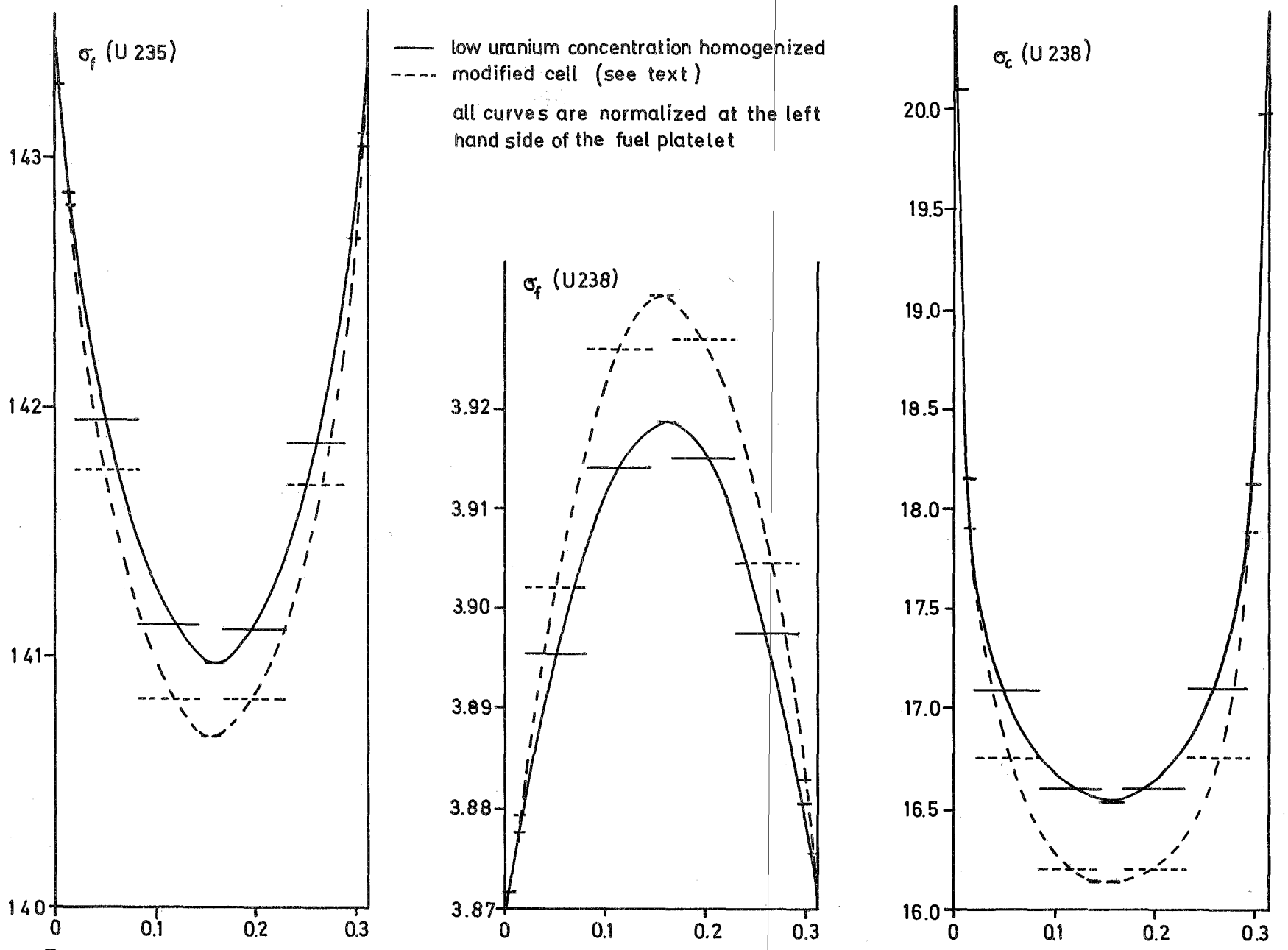


Fig. 5 Comparison of reaction rate taverses in the normal fuel platelet for different platelet arrangement in the normal cell

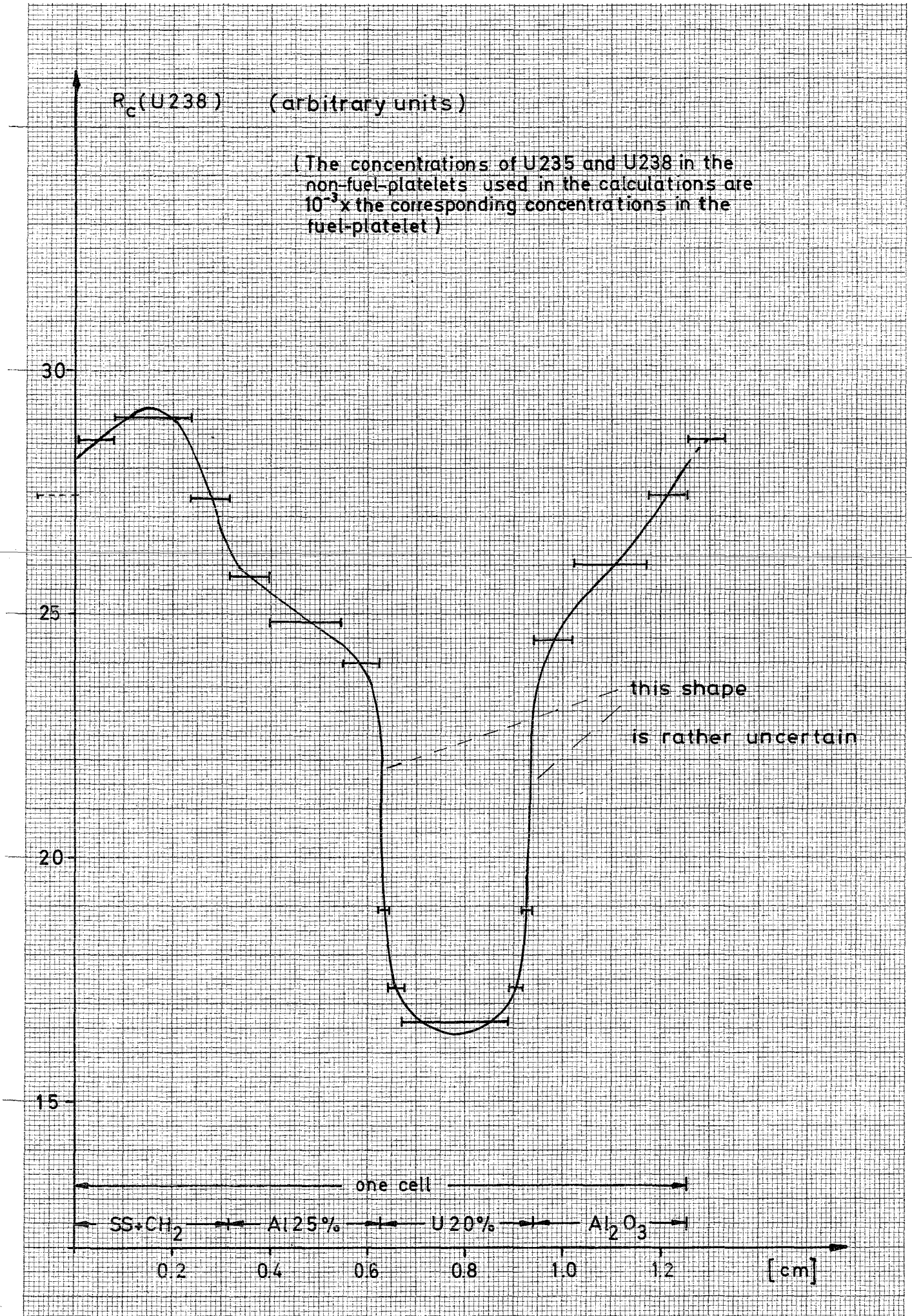


Fig. 6a. Microscopic reaction rate in the cell of SNEAK 3A2

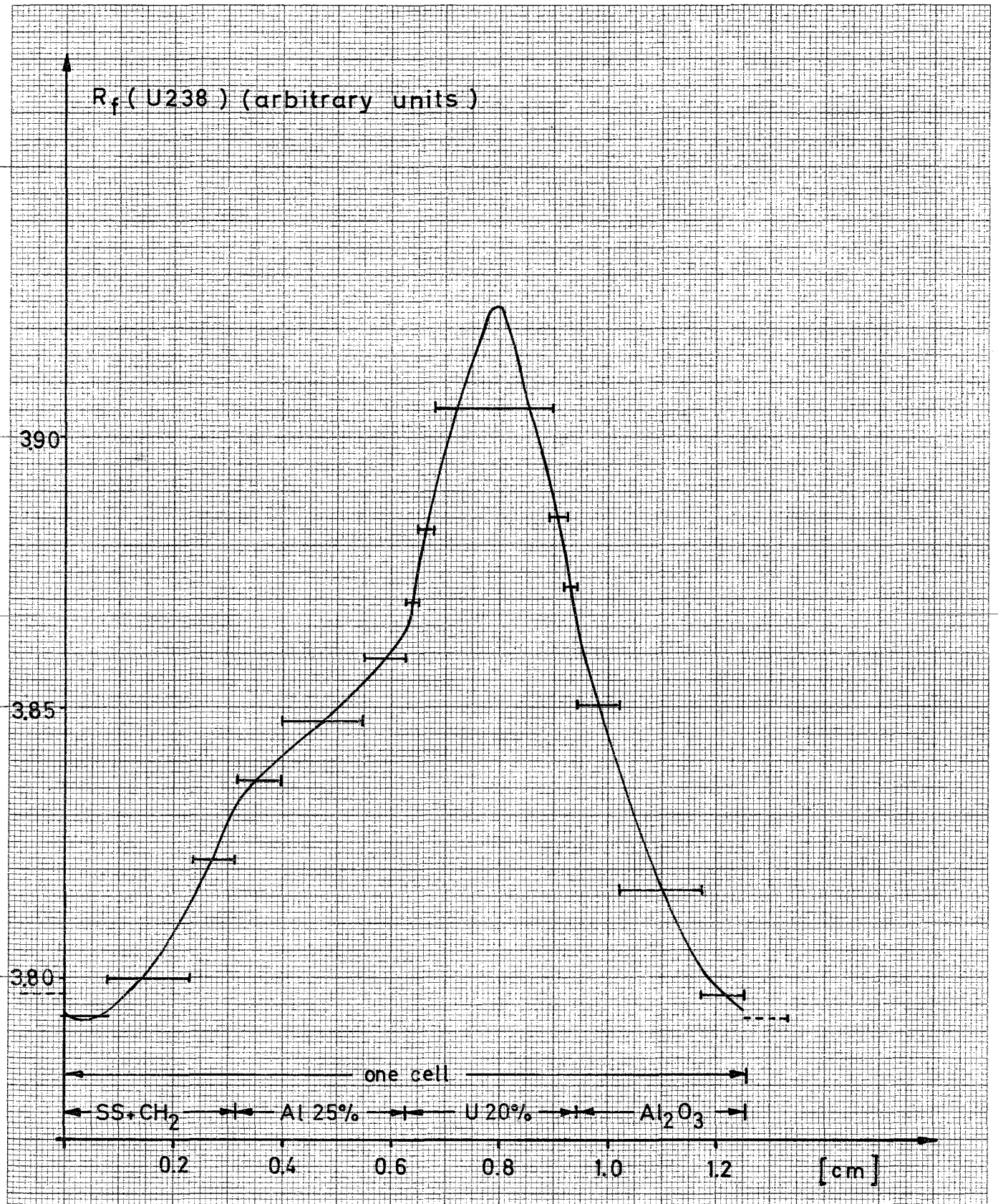


Fig.6b. Microscopic reaction rate in the cell of SNEAK 3A2

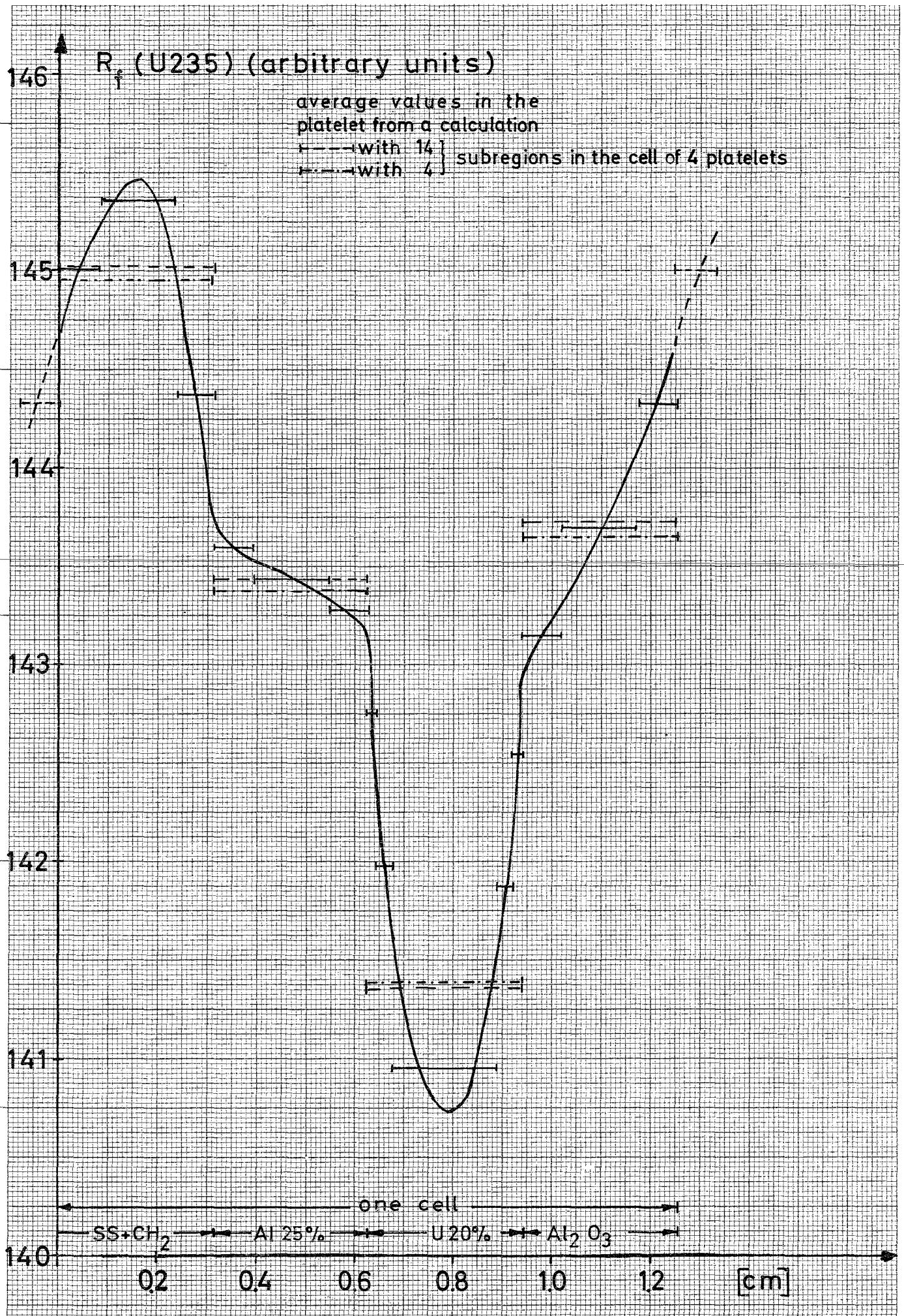
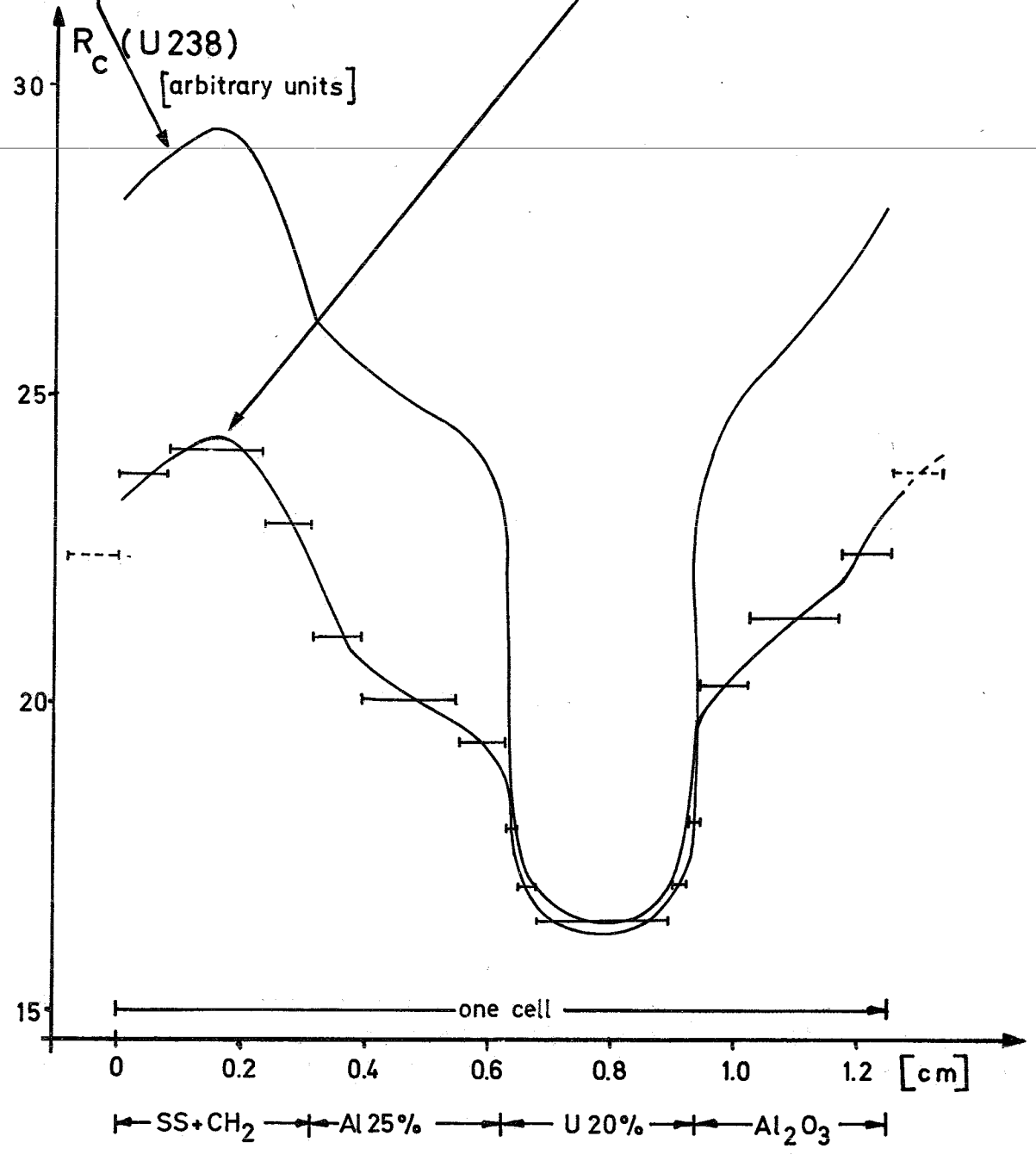


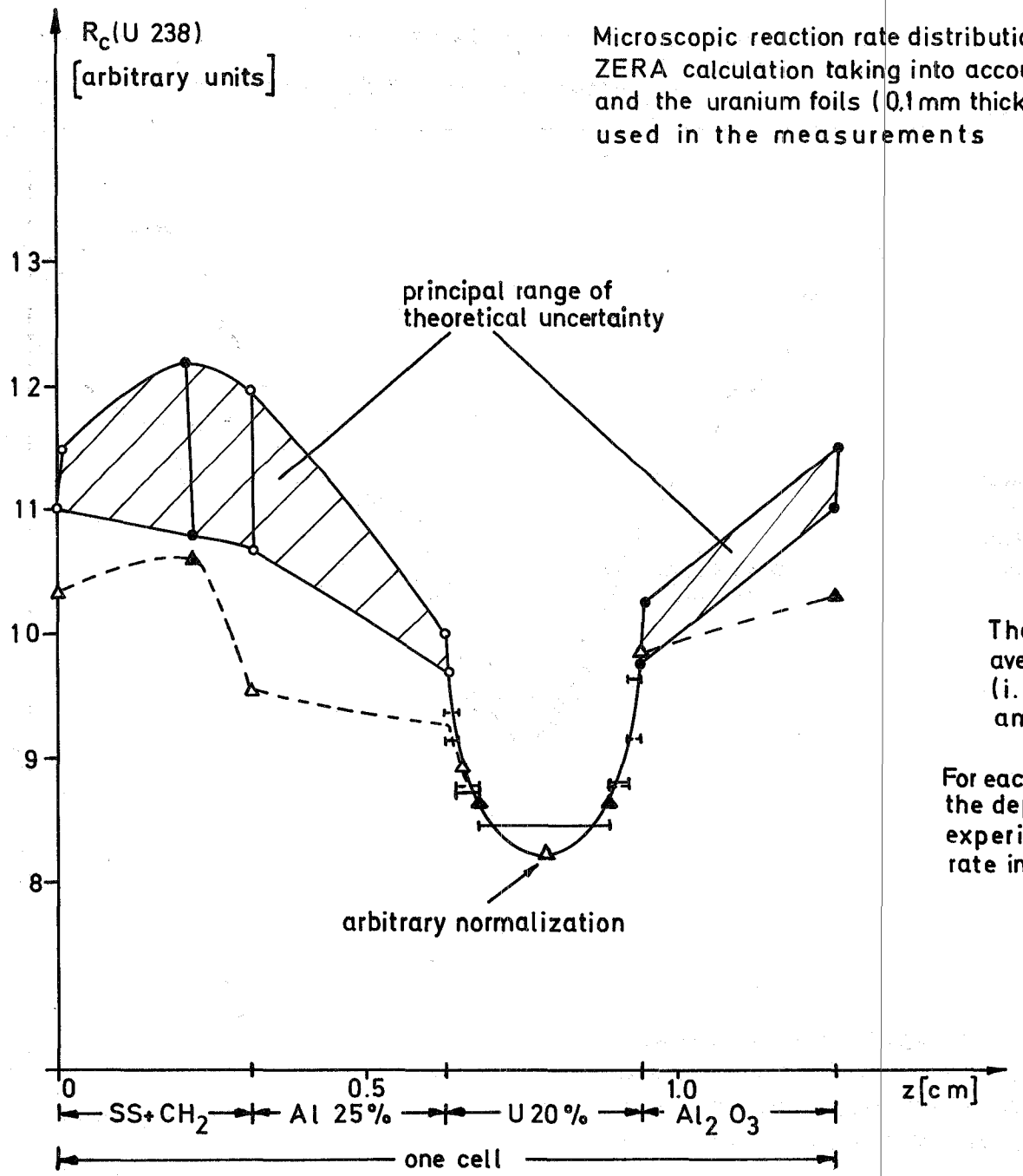
Fig.6c Microscopic reaction rate in the cell of SNEAK 3A2

Fig. 7

concentration of U 235 and U238 in nonfuel-platelets = 10^{-3} · concentration in the fuel platelet

the two uranium foils (0,44% and 20,04% enriched) are homogenized over each platelet to give the U235 and 238 concentrations in the non-fuel-platelets





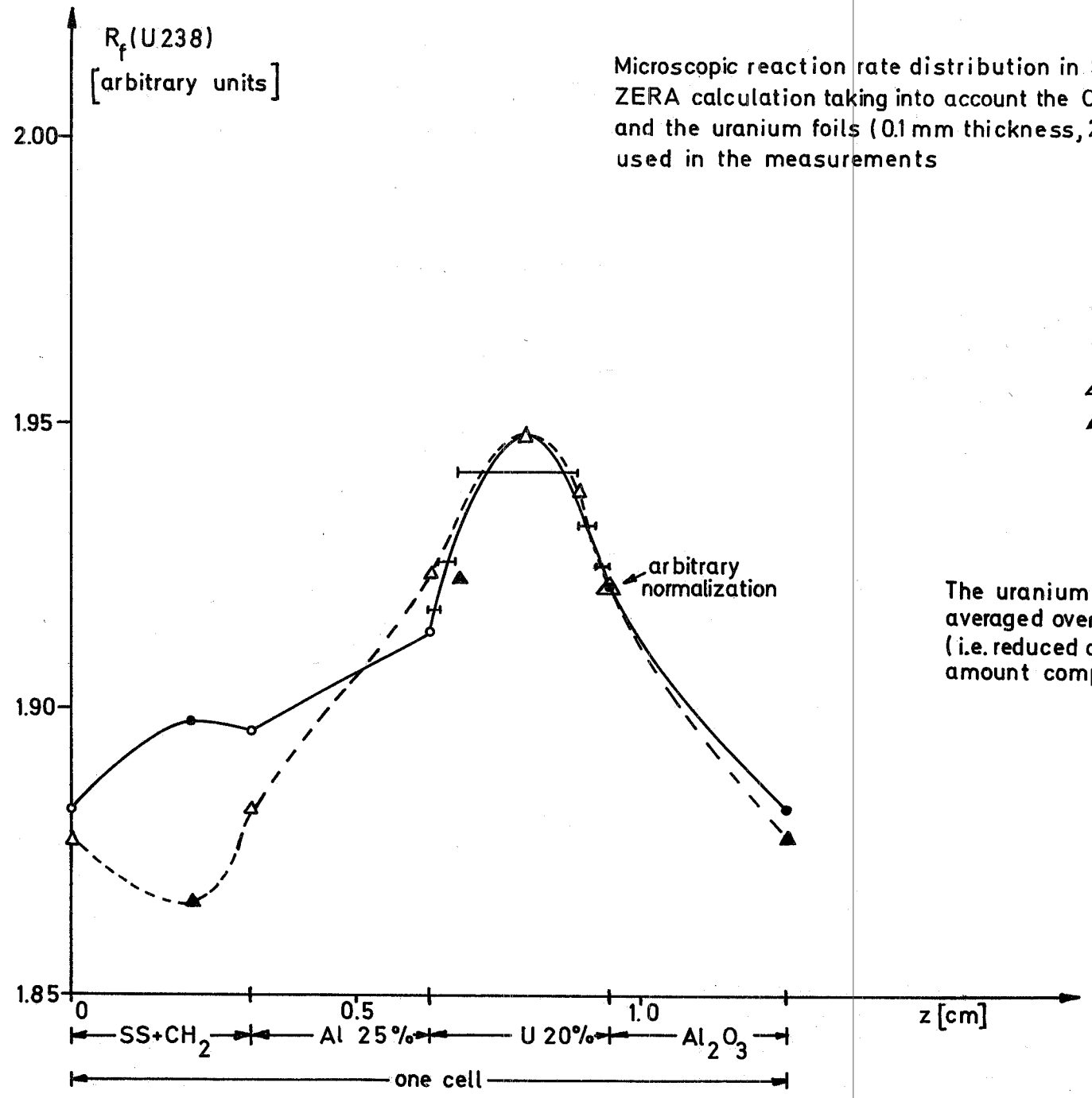
Microscopic reaction rate distribution in SNEAK 3A2 cell
ZERA calculation taking into account the CH_2-foil (41.x41.x0.5mm)
and the uranium foils (0.1mm thickness, 25.4mm diameter)
used in the measurements

- calculated for fuel-platelet
- calculated for fuel-platelet in adjacecent cell
- calculated for foils
- calculated for foils in adjacent cell
- measured with foils
- measured with foils in adjacent cell

The uranium foils of 0.1mm thickness have been averaged over the whole lattice area (544x544mm^2) (i.e. reduced concentration but correct total amount compared to reality)

For each pair of foils the one at the right hand side is the depleted uranium foil, which has been used in the experiments for the determination of the capture rate in U 238

Fig. 8a

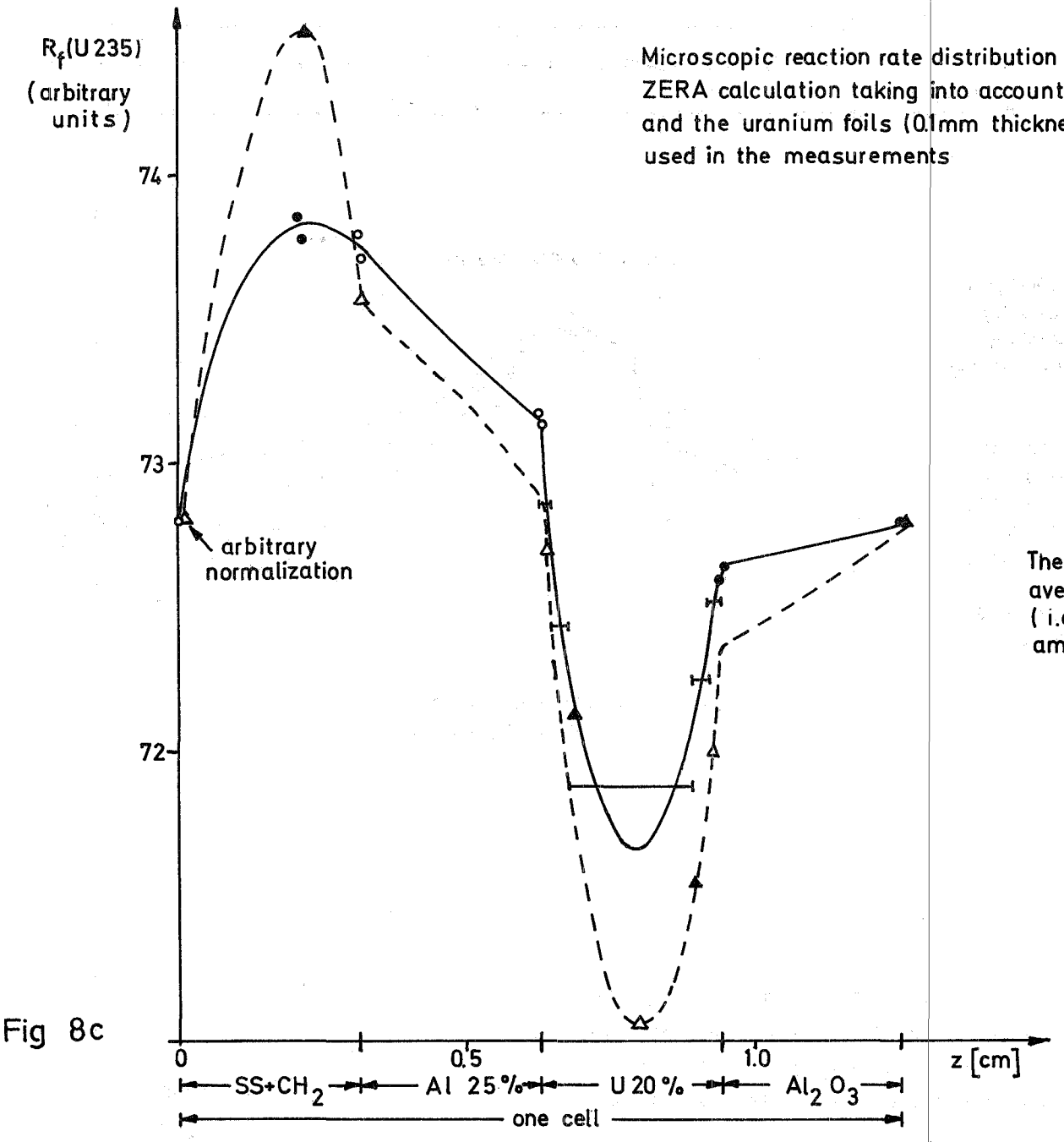


Microscopic reaction rate distribution in SNEAK 3A2 cell
ZERA calculation taking into account the CH_2-foil (41.x41.x0.5mm)
and the uranium foils (0.1 mm thickness, 25.4 mm diameter)
used in the measurements

- o calculated for foils
- ● calculated for foils in adjacent cell
- △ measured with foils
- ▲ measured with foils in adjacent cell

The uranium foils of 0.1mm thickness have been averaged over the whole lattice area (54.4x54.4mm^2) (i.e. reduced concentration but correct total amount compared to reality)

Fig. 8b



Microscopic reaction rate distribution in SNEAK 3A2 cell
ZERA calculation taking into account the CH_2 foil (41.x 41.x0.5mm)
and the uranium foils (0.1mm thickness, 25.4mm diameter)
used in the measurements

- ○ calculated for foils
- ● calculated for foils in adjacent cell
- △ measured with foils
- ▲ measured with foils in adjacent cell

The uranium foils of 0.1mm thickness have been averaged over the whole lattice area (54.4 x 54.4 mm^2) (i.e. reduced concentration but correct total amount compared to reality)

Fig 8c

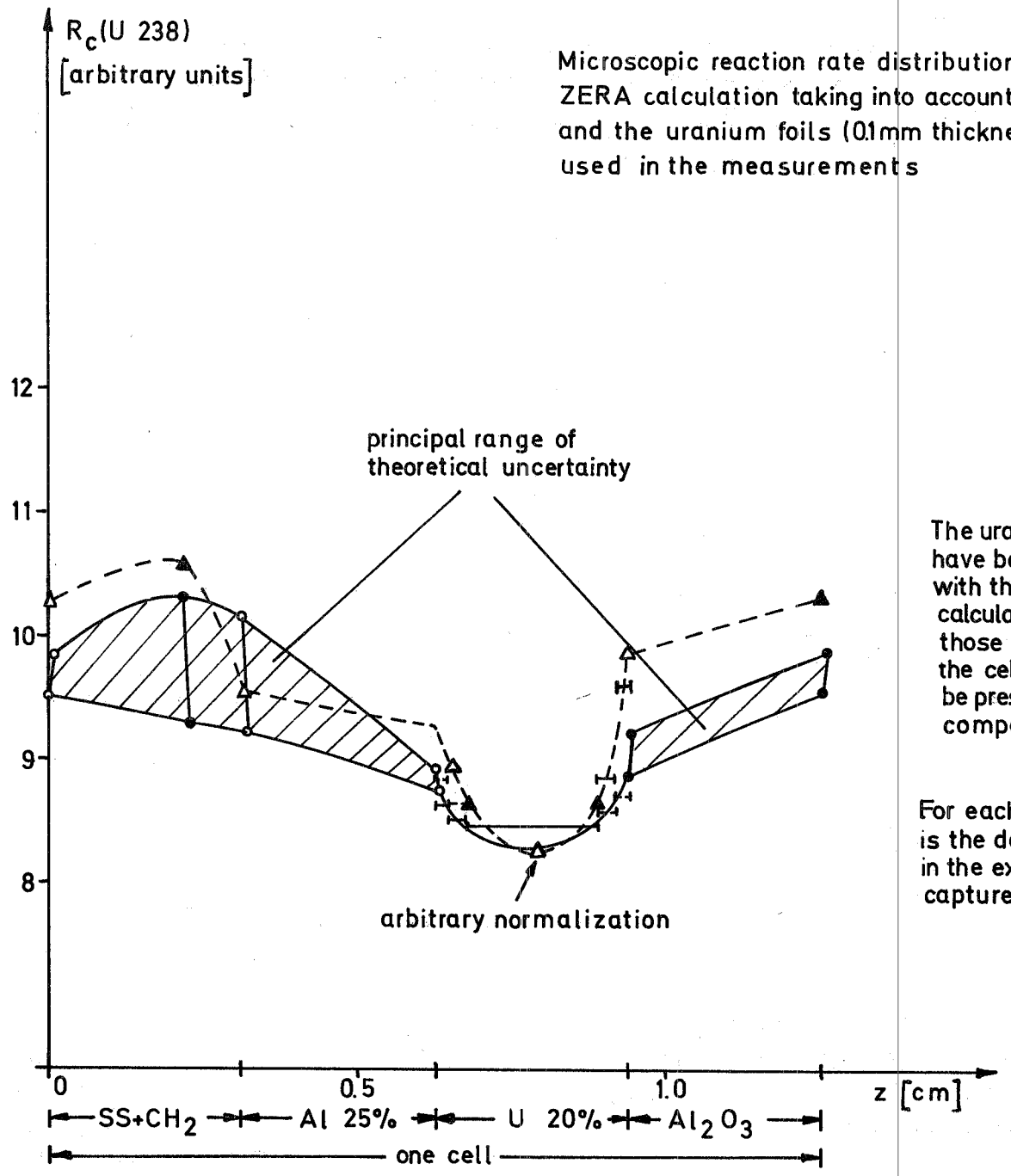


Fig. 9

Microscopic reaction rate distribution in SNEAK 3A2 cell
ZERA calculation taking into account the CH_2-foil (41.x41.x0.5 mm)
and the uranium foils (0.1 mm thickness, 25.4 mm diameter)
used in the measurements

- calculated for fuel-platelet
- calculated for fuel-platelet in adjacent cell
- ○ calculated for foils
- ● calculated for foils in adjacent cell
- △ measured with foils
- ▲ measured with foils in adjacent cell

The uranium foils of 0.1 mm thickness and 25.4 mm diameter have been extended over the whole lattice area (54.4x54.4 mm^2) with the real concentrations present in the foils (i.e. in the calculations the concentrations in the foils correspond to those really present in the central part of the cell, near the cell axis, but the total amount of uranium assumed to be present in the foils is larger by a factor of 5.84 compared to reality)

For each pair of foils the one at the right hand side is the depleted uranium foil, which has been used in the experiments for the determination of the capture rate in U 238

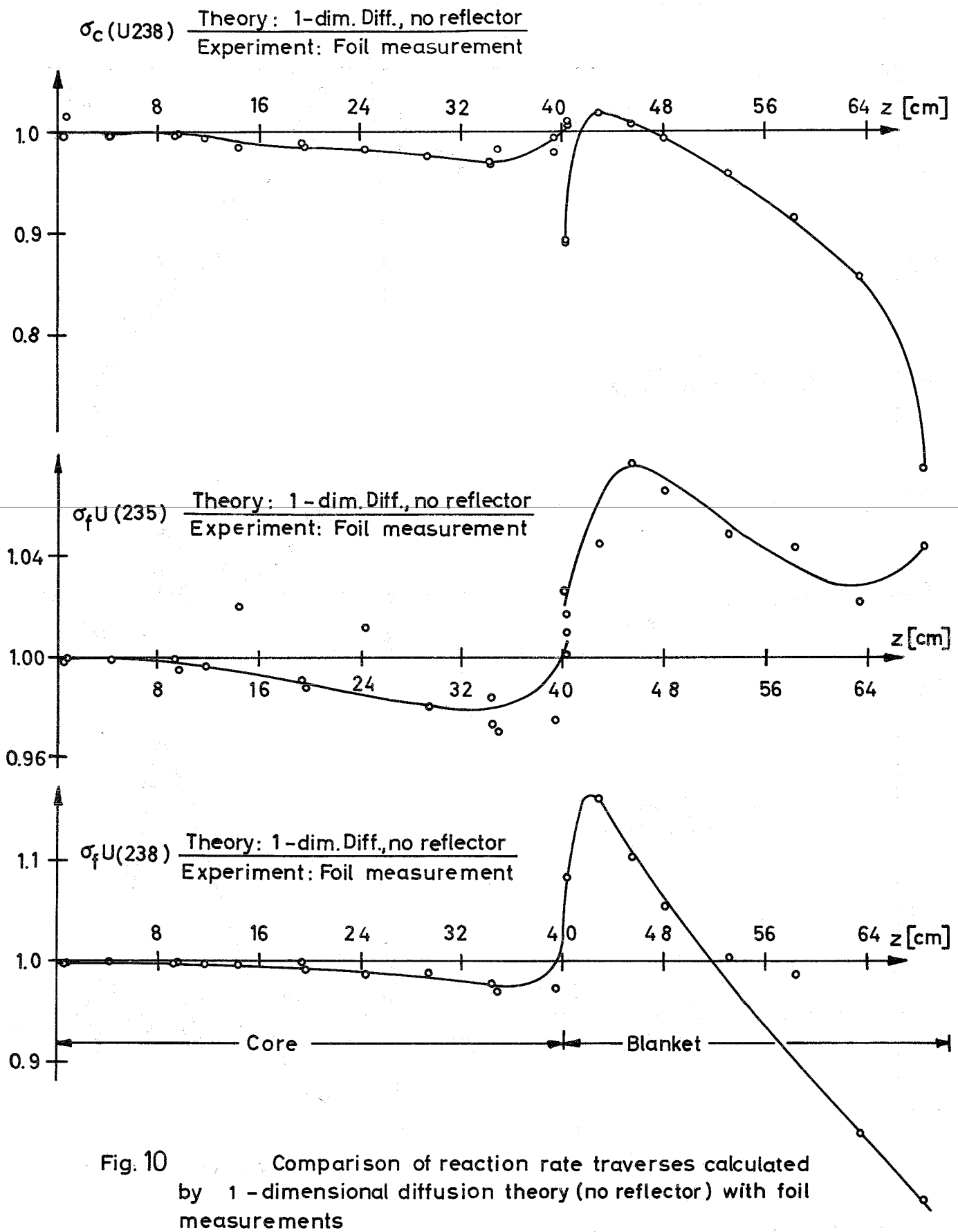


Fig. 10 Comparison of reaction rate traverses calculated by 1-dimensional diffusion theory (no reflector) with foil measurements

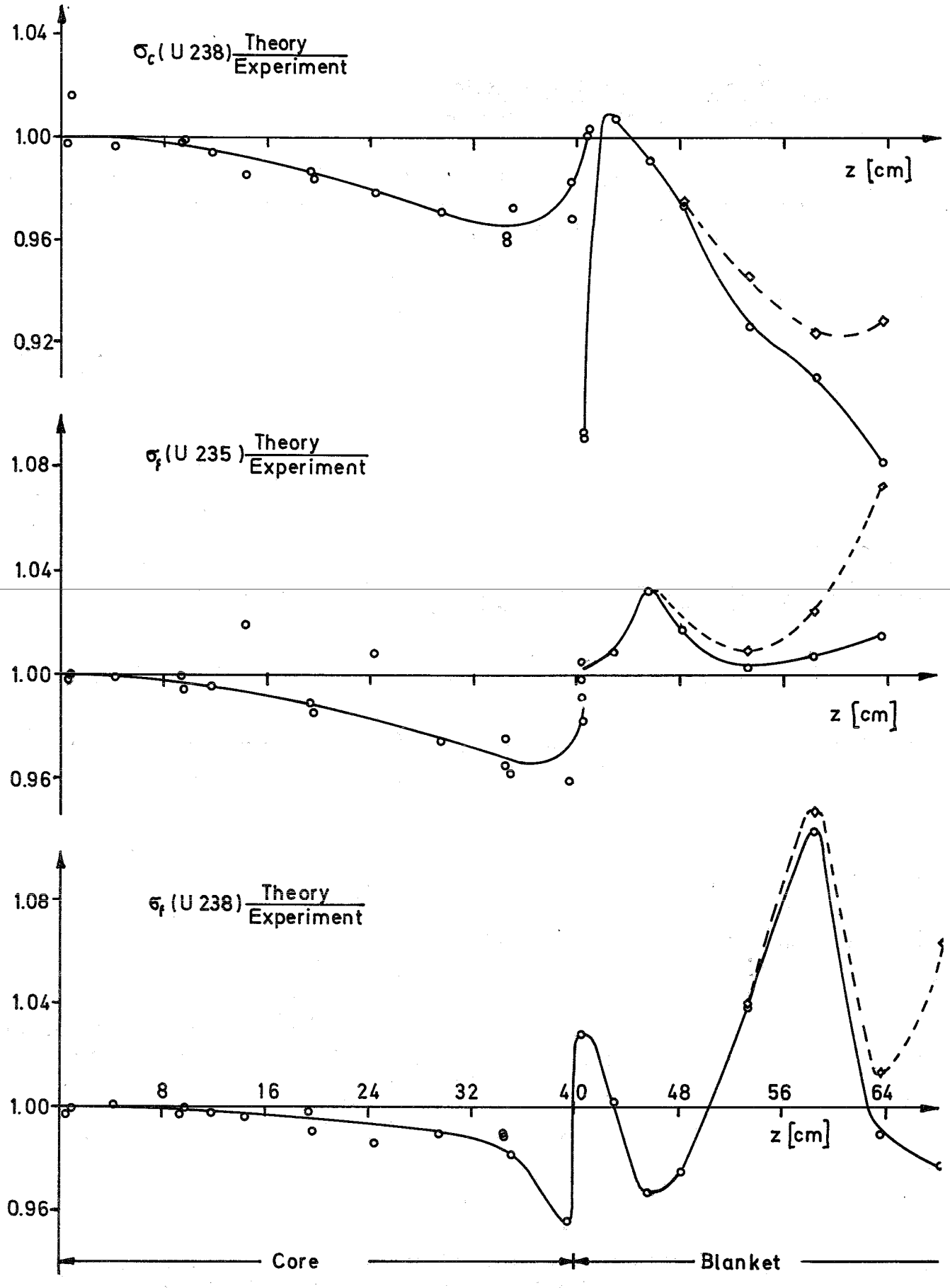


Fig. 11. Comparison of experimental reaction rate traverses with best available theoretical results without special consideration to the heterogeneity present at the core-blanket-interface

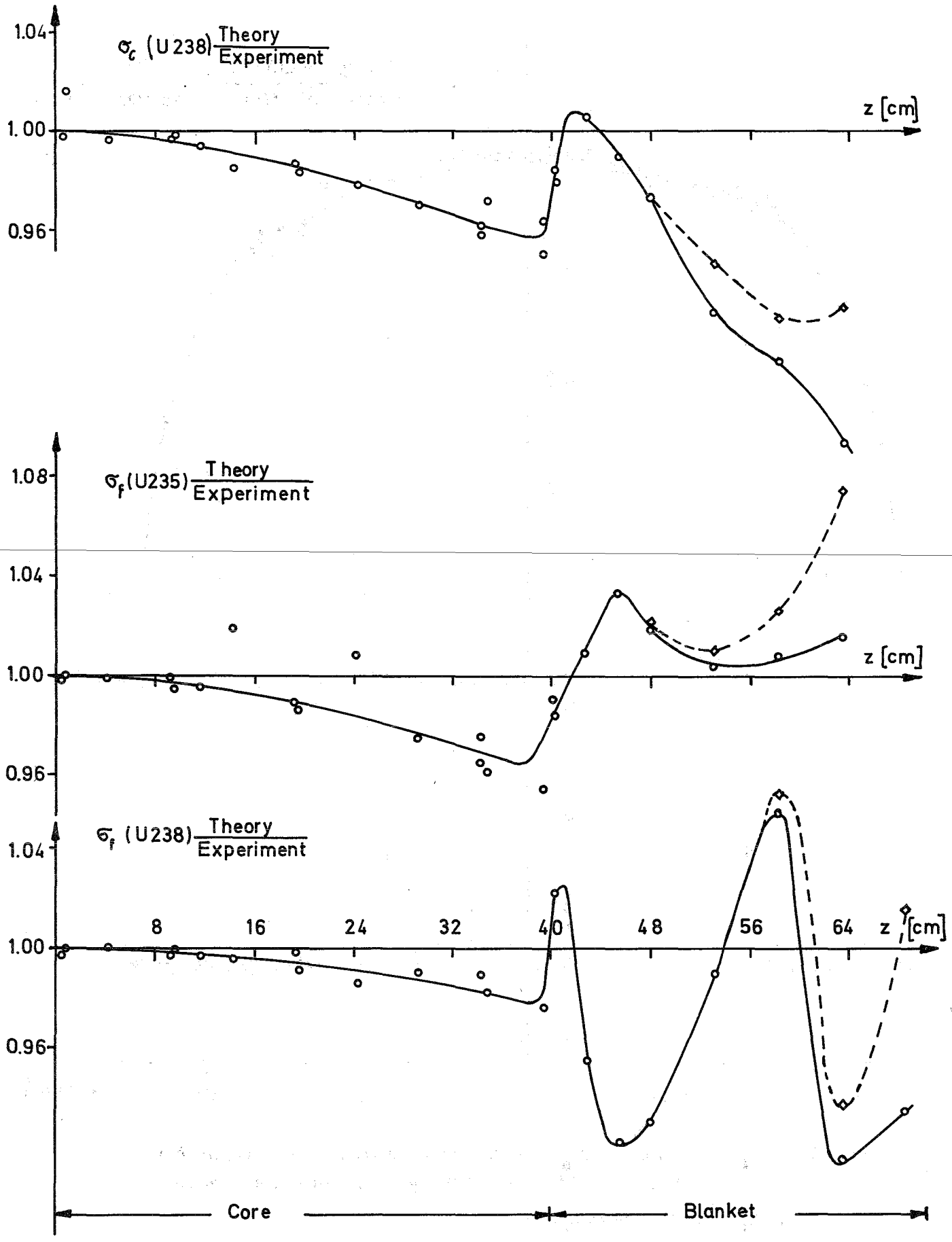


Fig. 12 Comparison of experimental reaction rate traverses with best available theoretical results taking into account the heterogeneity present at the core-blanket interface

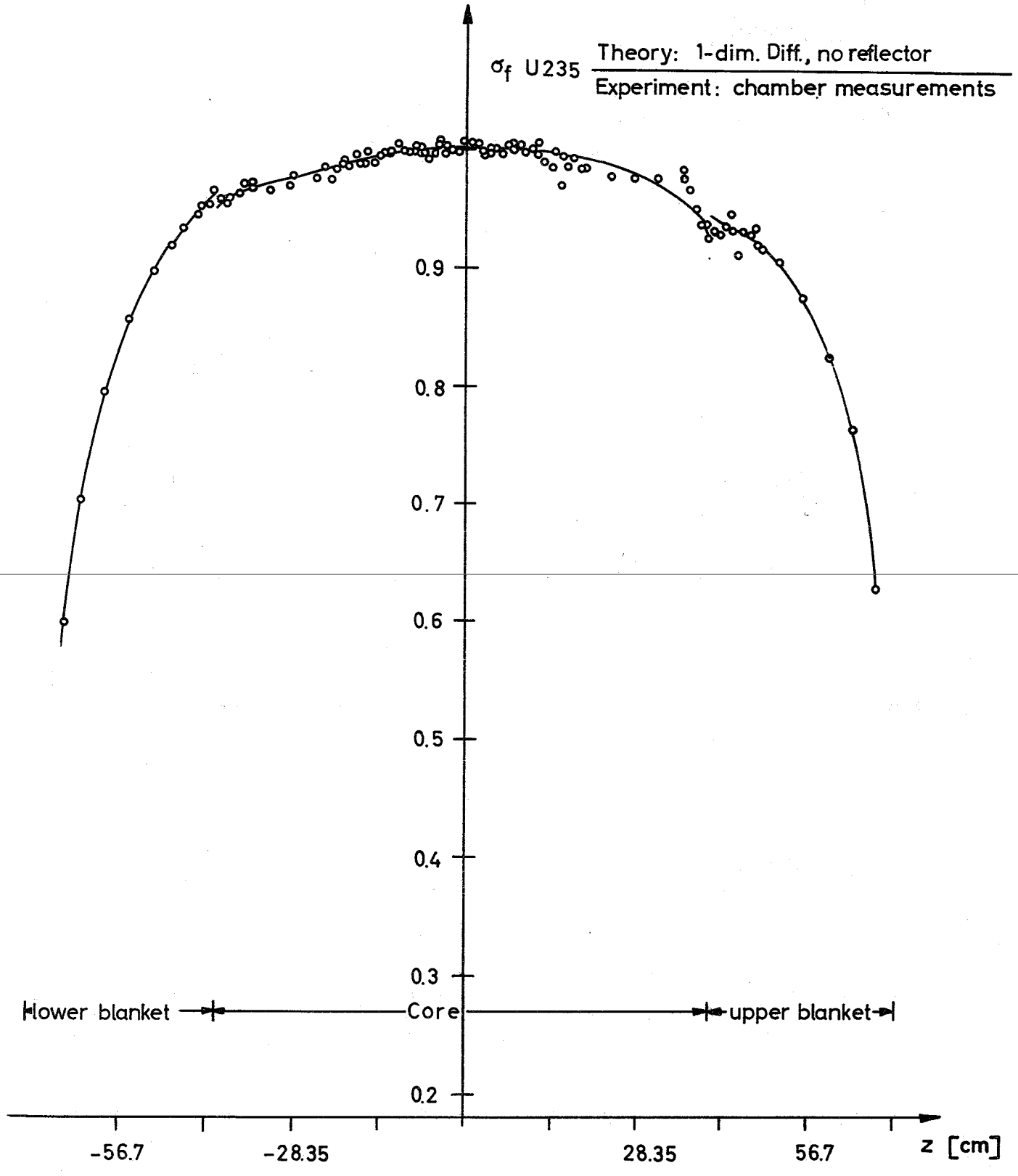


Fig. 13 Comparison of reaction rate traverses calculated by 1-dimensional diffusion theory (no reflector) with chamber measurements

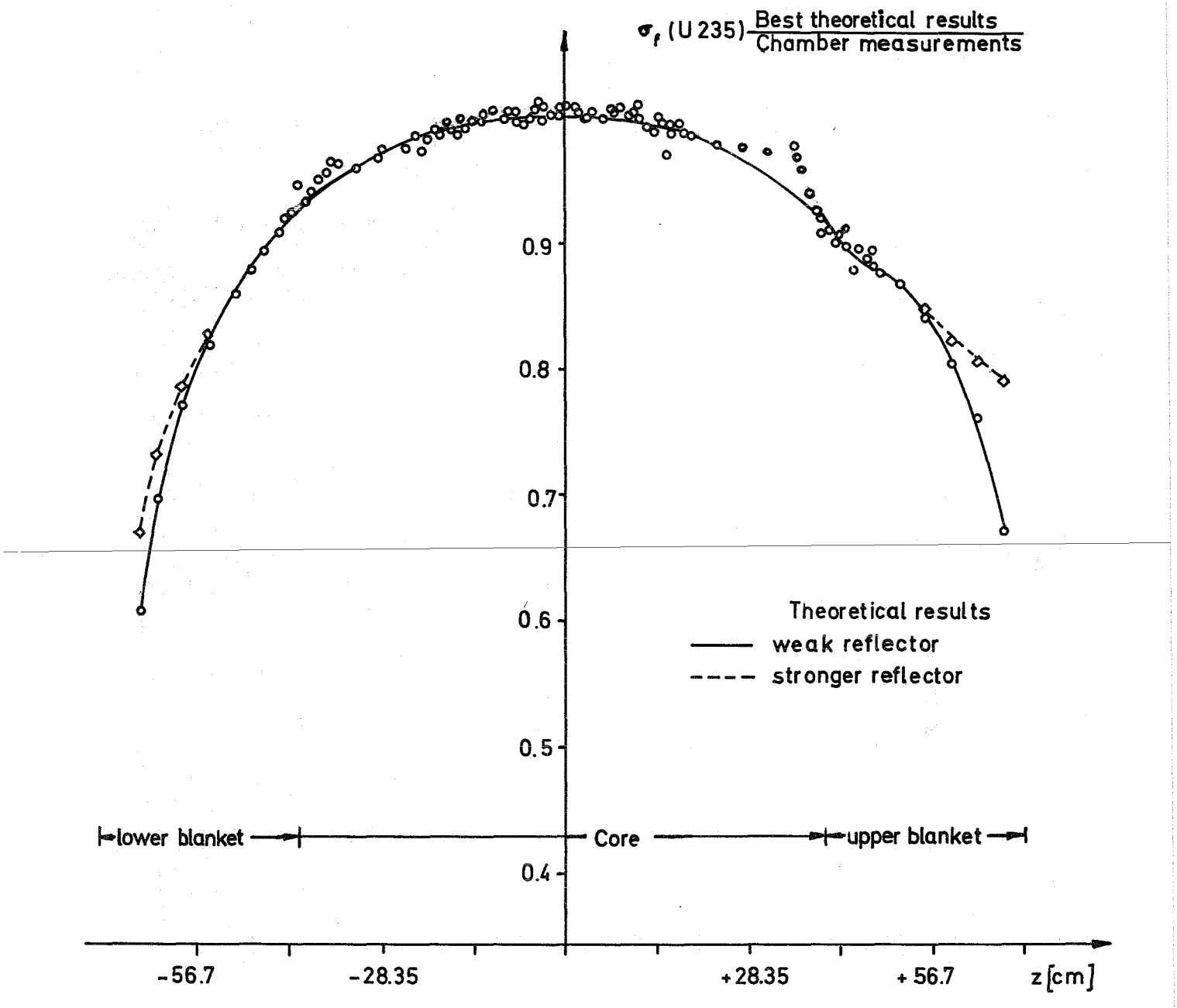


Fig.14 Comparison of best available calculated results for reaction rate traverses with the results of chamber measurements in SNEAK 3A2

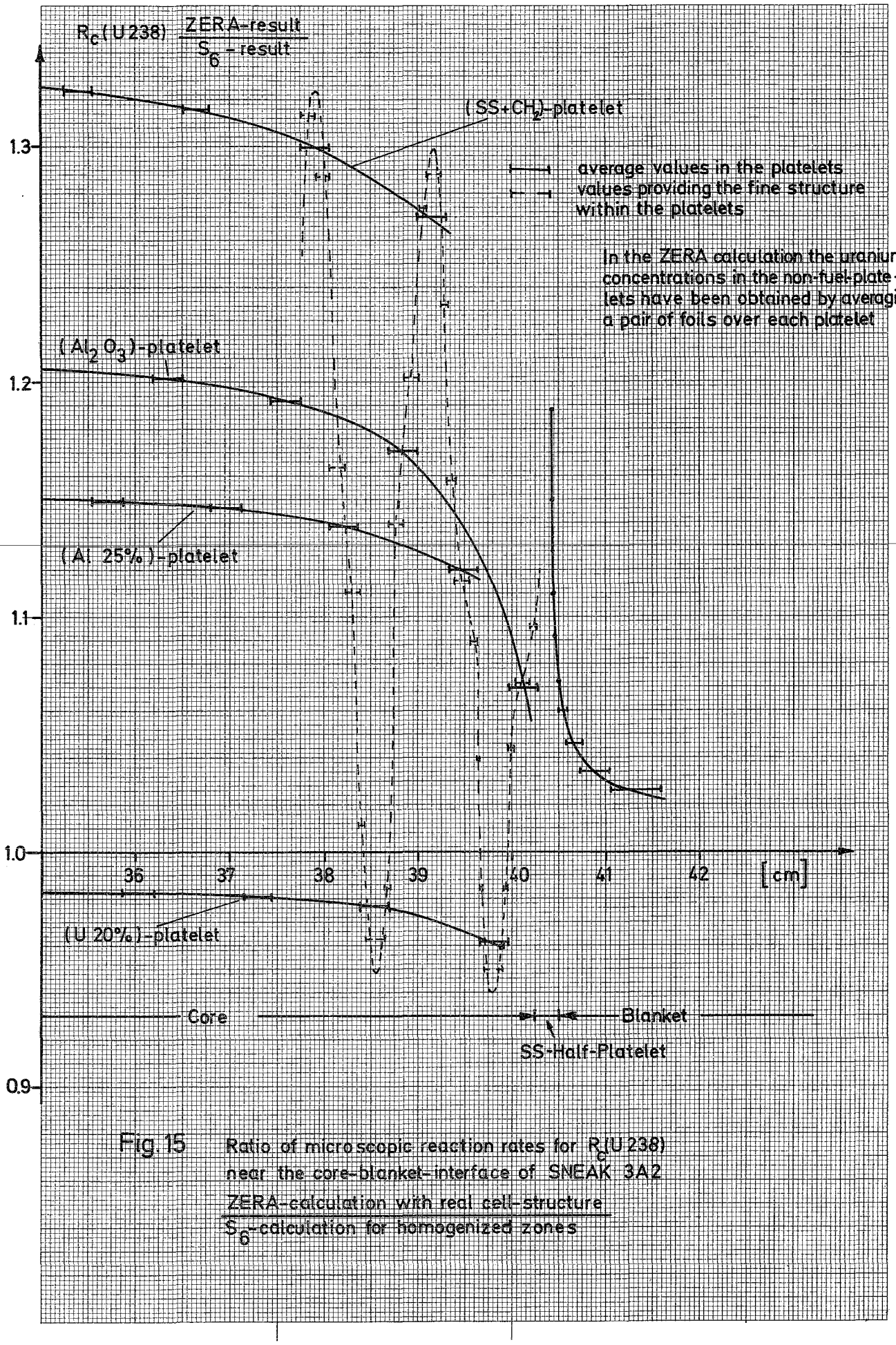


Fig. 15 Ratio of microscopic reaction rates for R_c(U238) near the core-blanket-interface of SNEAK 3A2

ZERA-calculation with real cell-structure / S_6-calculation for homogenized zones

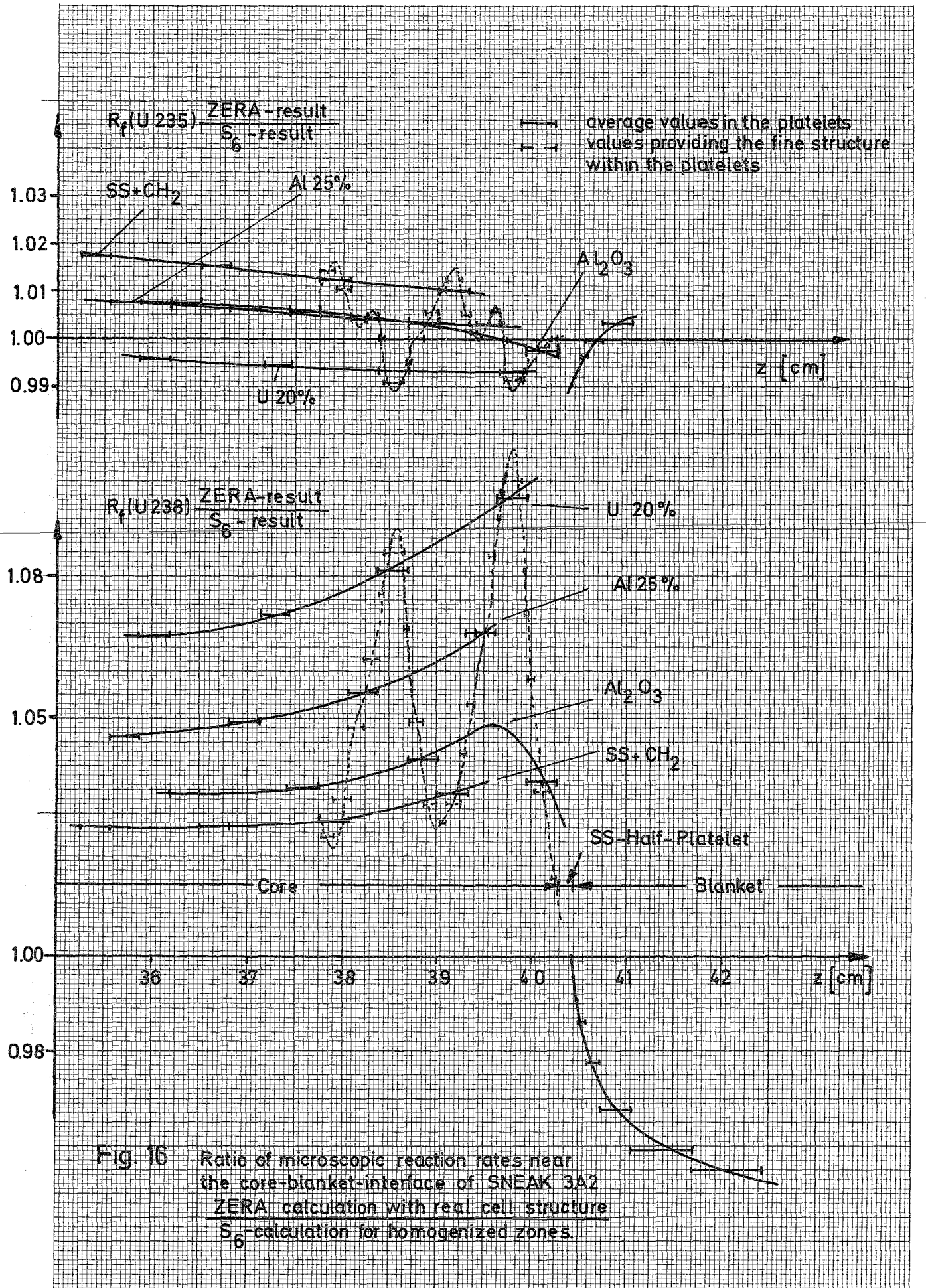


Fig. 16 Ratio of microscopic reaction rates near the core-blanket-interface of SNEAK 3A2

$\frac{\text{ZERA calculation with real cell structure}}{S_6\text{-calculation for homogenized zones.}}$

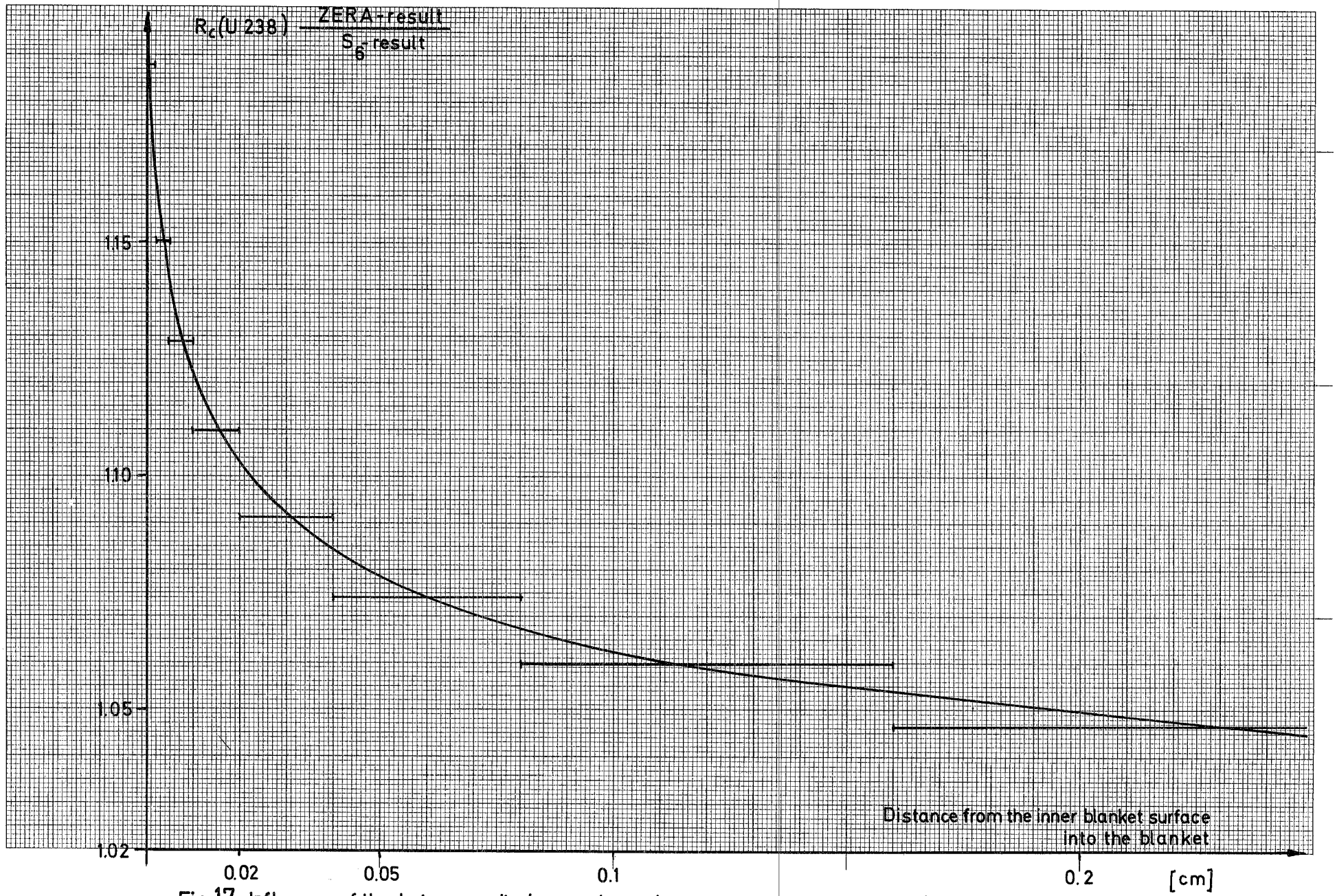


Fig.17 Influence of the heterogeneity (space dependent resonance self-shielding) on the U238 capture traverse in the inner part of the blanket of SNEAK-3A2