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Abstract

In his investigations concerning sodium void reactivities for SNEAK-9C2-assemblies Ganesan detected inconsistencies in the results coming from Δk of successive diffusion and exact perturbation calculations, respectively. Therefore, in this study discretization and rounding errors in neutronic reactor calculations and their effects on numerical results are considered for a well known SNR-300 type benchmark problem as well as for the slightly simplified original problem.

The main conclusions which can be drawn from the results of the present calculations are as follows (the first three refer mainly to the presently at KfK available DIXY version):

1) The inconsistencies for small mesh steps have their origin in the single precision of internal data representation of the programme DIXY-KfK, used by Ganesan for his investigations.

2) Mesh refinements do not necessarily lead to an improved accuracy of the results because the decreasing of discretization error is eventually more than counterbalanced by an increasing rounding error.

3) The accuracy of results for the determination of the sodium void and other reactivity effects of small absolute magnitude obtained from successive criticality calculations may not in all cases be improved by a reduction of the mesh size. For those cases where a mesh refinement leads to a deterioration of the reliability of criticality differences results obtained from perturbation calculations are much more reliable and fairly insensitive to the mesh size as has also been shown by Ganesan.

4) Comparisons of the IBM-version DIXY-KfK and the corresponding CDC-version DIXY-IA (with an internal data representation nearly equivalent to a double precision IBM version) showed that there exists an optimum value for the mesh size leading to the best accuracy attainable by DIXY-KfK for k_{eff}. For control rod worths and sodium void effects recommendations have been derived for mesh sizes which should not be exceeded in order to keep the numerical uncertainties below reasonable specified limits.

Einfluß der Maschenweite auf die Ergebnisse von Diffusionsrechnungen für Schnelle Brutreaktoren

Zusammenfassung

Ganesan stellte bei Untersuchungen zur Berechnung des Natrium-Void-Reaktivitätskoeffizienten für SNEAK-9C2-Anordnungen Inkonsistenzen zwischen den Reaktivitätswerten fest, die aus der Differenz zweier Kritikalitätsrechnungen bzw. als Ergebnis einer exakten Störungsrechnung bestimmt wurden. Davon ausgehend werden in dieser Studie die Auswirkungen von Diskretisierungs- und Rundefehlern auf die Ergebnisse von Neutronik-Diffusions-Rechnungen anhand eines für den SNR-300 typischen Benchmarkproblems und eines Modells untersucht, das gegenüber dem von Ganesan betrachteten Problem geringfügig vereinfacht wurde.

Dabei ergaben sich die folgenden Ergebnisse (die Punkte 1) - 3) beziehen sich hauptsächlich auf die im KfK verfügbare DIXY Version):

1) Die Ursache für die von Ganesan beobachteten Inkonsistenzen in den Ergebnissen liegt in der Verwendung einfacher Genauigkeit für die interne Zahlendarstellung bei dem für die Untersuchungen verwendeten Rechenprogramm DIXY-KfK.

2) Schrittweitenverfeinerungen führen nicht notwendigerweise zu einer verbesserten Genauigkeit der Ergebnisse, weil eine Verkleinerung des Diskretisierungsfehlers möglicherweise durch eine Vergrößerung des Rundefehlers mehr als ausgeglichen wird.

3) Die Bestimmung von Natrium-Void- und anderen Reaktivitätseffekten mit kleinen absoluten Werten aus Differenzen zweier Kritikalitätsrechnungen kann auch für kleine Schrittweiten zu ungenauen Resultaten führen. In solchen Fällen sind die Ergebnisse aus Störungsrechnungen wesentlich zuverlässiger und nahezu unabhängig von der Größe der gewählten Schrittweiten, wie dies auch von Ganesan gezeigt wurde.

4) Vergleichsrechnungen zwischen der IBM-Version DIXY-KfK und der entsprechenden CDC-Version DIXY-IA (mit einer internen Zahlendarstellung, die etwa der doppelten Genauigkeit der IBM-Version entspricht) zeigten,

daß für die Schrittweite ein optimaler Wert angegeben werden kann, mit dem bezüglich k_{eff} die höchste, mit DIXY-KfK erreichbare Genauigkeit, erzielt werden kann. Für die Berechnung von Kontrollstabwerten und Natrium-Void-Reaktivitätskoeffizienten werden obere Grenzen für die zweckmäßigerweise zu wählenden Schrittweiten angegeben, die im Hinblick auf die gewünschte numerische Genauigkeit nicht überschritten werden sollten.

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I Introduction

In investigating sodium void reactivities for the assembly SNEAK-9C-2, Ganesan /1/ detected inconsistencies in the results coming from Δk of successive diffusion or exact perturbation calculations and he demands for a decision which one of both methods can be considered as more reliable. Ganesan performed the Δk calculations by the Karlsruhe version of the 2-d diffusion code DIXY /2/. Benchmark calculations /3,4/ demonstrated that this version of DIXY-KfK leads to inconsistencies in the results for k_{eff} using small mesh steps.

In the meantime the benchmark calculations have been repeated using the Interatom version of DIXY-IA.* Both versions mainly differ in the computer internal representation of data. DIXY-IA uses a word length of 60 bits, corresponding to 14 reliable digits of a number, on the Cyber 172 instead of 32 bits on the IBM 370/168 of DIXY-KfK corresponding to 6 reliable digits.

The results obtained by DIXY-IA are considered to be reliable for two reasons:

A) The k_{eff} values obtained by DIXY-IA as a function of the mesh size show the expected linear behaviour whereas the results obtained by DIXY-KfK do not.

B) The discrepancies between the DIXY-IA and CITATION /5/ results for the mesh step going $\to 0$ are very small, this means less than $5 \cdot 10^{-5}$.

A detailed discussion of these properties will follow later on.

Therefore two activities have been pursued:

a) The benchmark problem in x-y-geometry calculated by DIXY-KfK dealing essentially with criticality values k_{eff} has been extended to investigations of the accuracy of control rod worths and sodium void reactivities dependent on mesh sizes. These results have been compared with those obtained by DIXY-IA in order to get some insight into the effects of rounding errors and to get more reliable values on the influence of the mesh size.

b) The Ganesan SNEAK-9C-2/POZ problem in r-z-geometry originally solved for 26 energy groups has been recalculated with DIXY-KfK.

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* At Interatom the CDC-version DIXY-IA has been derived from the original IBM-version DIXY-KfK.

The mesh size has been reduced systematically to fairly small values to determine its influence on k_{eff} and Δk. To reduce computing time only a 4 group representation has been used.

The present study should try to answer the following questions related to the possible existence of unavoidable uncertainties (i.e. of intrinsic restrictions with respect to the attainable numerical accuracy) for criticality and reactivity values determined by the present version of DIXY-KfK:

1) Is the single precision of internal data representation on the IBM 370/168 available at KfK mainly responsible for the inconsistencies of the DIXY-KfK results for the benchmark problem as well as for the Ganesan problem for small mesh steps?

2) To what extent can the numerical accuracy and reliability of the DIXY-KfK results be improved by a mesh refinement? Does the influence of the rounding errors prevent taking full advantage of the reduction of the discretization error attainable with a mesh refinement?

3) Does there possibly exist an optimum mesh size with respect to the optimum numerical accuracy for a certain quantity (e.g. k_{eff}, control rod worth, sodium void effect) which can be obtained with the present single precision version of DIXY-KfK? The existence of such an optimum choice for the spatial discretization, leading to steps of the order of several cm, could be imagined because the decreasing discretization error correlated with a reduction of the mesh size might be counterbalanced by an increasing rounding error.

4) Is it possible to give some advice with respect to the reliability of reactivity effects deduced from successive criticality calculations?

5) What conclusions can be drawn from a comparison of sodium void reactivities determined from successive k_{eff}-calculations and exact perturbation calculations, respectively? Is it possible to decide which method is the more reliable one and, therefore, should be recommended for future studies of the same kind as performed by Ganesan /1/?

II General Considerations concerning the Accuracy and Reliability of Calculated Results

The results of reactor calculations are usually influenced by a multitude of uncertainties and inaccuracies. They are caused by a lot of sources as for example:

1) Uncertainties in the measured and evaluated basic data, and correspondingly in the macroscopic neutron cross sections.

2) Approximations for the computational model. The time independent Boltzmann neutron transport equation, describing the neutron flux distribution as a function of six variables for the neutron energy, space- and angle-coordinates is the basis for all static reactor calculations. Due to restrictions in computing time and the corresponding lack of very sophisticated computer programs it is usually impossible to treat the neutron transport process in all details with respect to its dependence on the six variables mentioned before. This means that one cannot follow the neutron paths in the six-dimensional space as closely as desirable. The solution is in general only possible if we restrict its solution domain to a certain subspace of the complete domain. The corresponding approximations and simplifications which have to be introduced can be considered in a mathematical sense as some kind of projection operators. They have to be applied for several reasons and purposes:

   a) Analytical solutions of the neutron transport equation are scarce and restricted to specific problems which are usually not typical for practical applications. But even in these more academic cases the numerical evaluation may become complicated. Therefore, assuming a certain approximation for the relationship between the neutron flux and the neutron current, the neutron transport equation is often reduced to the neutron diffusion equation.

   b) The distribution of the neutron number density is a fairly complicated function of the neutron velocity or the neutron energy. An appropriate representation would require at least several thousands of energy points or energy intervals in order to resolve the resonances of the materials comprising the main components (e.g. Na, Fe,

^{238}U, ^{239}Pu) of the core compositions. For practical applications the number of energy groups is usually smaller than about 30.

c) The neutron interaction with the materials appearing in the various compositions of a complicated reactor configuration is described by group cross sections corresponding to a chosen energy group structure mentioned before. In principal, the exact energy dependent solution for the neutron number density has to be known to derive these group cross sections (or group constants). In practice, certain approximations are applied so that, using a given energy dependent weighting function, these group constant data can be evaluated in tabular form. For the actual application the effective group constants for the individual compositions or material mixtures can then be obtained from these tabulated data. Sometimes some iterative procedure is applied to improve the effective group constants, this being an indication of the fact that the exact solution should be known in advance to the derivation of group constants.

d) Even if we restrict ourselves to the so-called multigroup neutron diffusion equation, we have to be aware that analytical solutions are possible only for a small number of special examples. Since these are usually not sufficient for practical purposes, discretization of space variables is indispensable for the solution of the diffusion equation for normal reactor configurations or test facilities.

e) The solution of the neutron diffusion equation is also very time-consuming for most of the problems under consideration. The original 3-dimensional problem is therefore frequently reduced to two- or even one-dimensional problems by suitably remodelling the original configuration or by handling the missing space dimension with a buckling concept.

3) Uncertainties in the transformation of the original, usually complicated physical problem into a simplified mathematical model. There exist different prescriptions or recipes (homogenization procedures) for transforming the real configuration into a similar but more crude and more homogeneous model suitable for the desired numerical treatment.

4) Numerical uncertainties such as rounding errors.

Disregarding all other sources of uncertainties, in this study only those effects are considered which influence the accuracy of criticality values determined with numerical methods caused by

- discretization effects (e.g. the mesh size)
- rounding errors.

Systematic investigations on the influence of these reasons on the final results for typical LMFBR configurations are scarce.

III Results for the SNR-300 Benchmark-Problem

As noted in /1/ the 2-dimensional diffusion code DIXY-KfK /2/ at present operates at Karlsruhe with a single precision representation of data on an IBM 370/168 computer. An indication of the influence of the special discretization scheme (by investigating mesh refinements) and especially of the rounding errors caused by the restricted word length of data can be found in the results of benchmark studies /3,4/: The DIXY-KfK results presented in /3/ and /4/ do not show the nearly linear dependence of k_{eff} as a function of the average area per mesh size in contrast to the expected behaviour observed for all other codes applied within that intercomparison and in contrast to the results of other studies e.g. /6/.

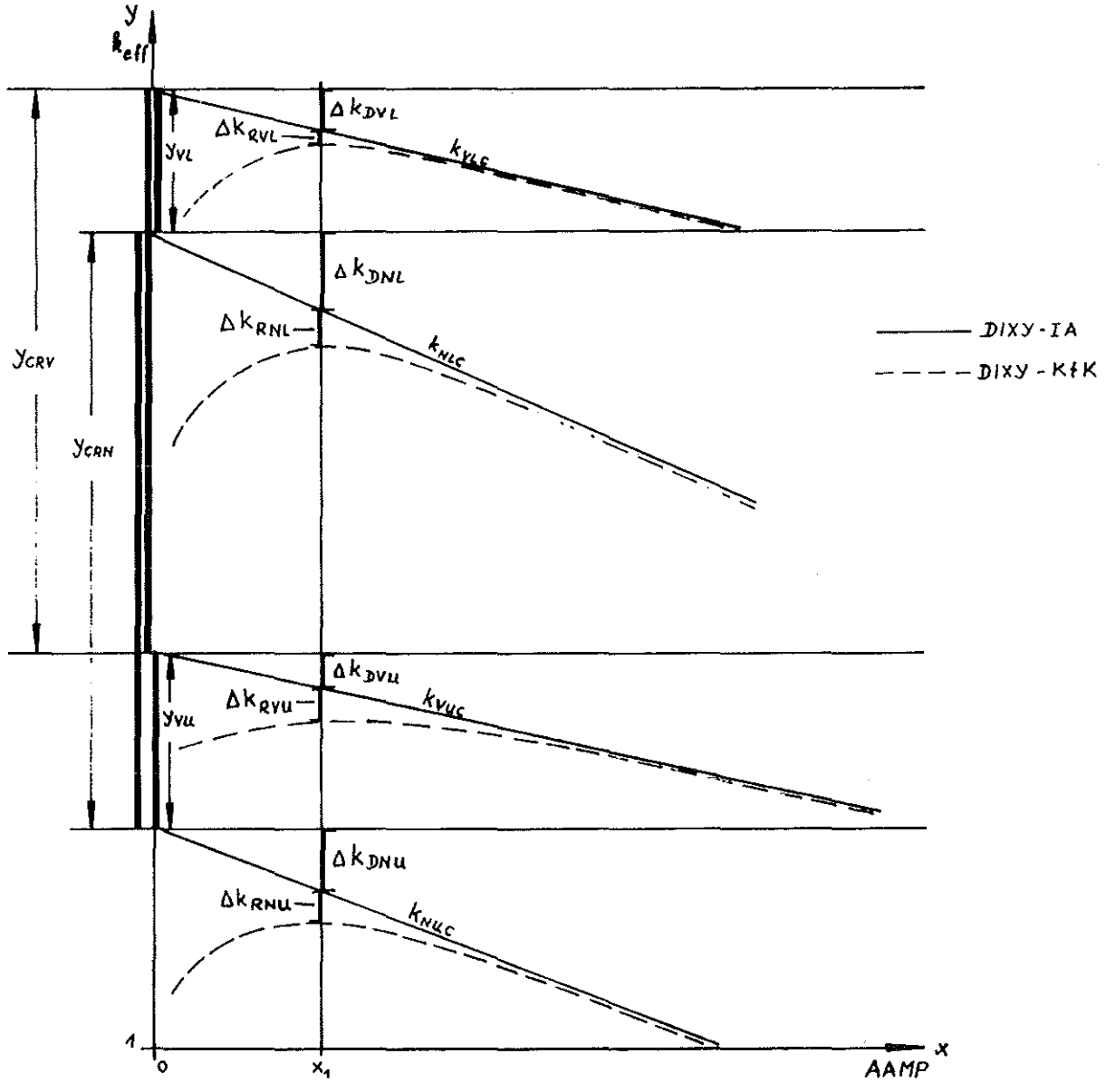
Therefore it seemed obvious that these benchmark activities could be a meaningful basis and starting point for studies aimed to determine the influence of discretization and rounding errors on the results for k_{eff}, control rod worth and sodium void reactivity. The investigations primarily concerned the xy-benchmark configurations which may be considered as representative examples for LMFBR horizontal core cross sections.

According to the classification used in /3/ we call model B1 the 2-d mesh grid with 20*20 space points. The mesh step of 5.4 cm in this model is equal to half the size of the subassemblies, represented in xy-geometry. Model Bi is obtained from B1 by dividing this mesh step by i. The number of mesh points resulting from this simple concept has to be slightly modified to accommodate the restriction of DIXY which requires the number of mesh points in at least one coordinate direction to be a multiple of four. So the mesh in the outer radial blanket region is slightly different from that described above. This means that the general mesh steps for the models B1 - B4 are attached to the following values of average area per mesh point (AAMP used in /3/, /4/ and /6/ and defined as the area of one horizontal plane out of the reactor problem divided by the number of mesh points in that plane).

model	general mesh step (cm)	AAMP (cm^2)
B1	5.4	27.72
B2	2.7	6.93
B3	1.8	3.08
B4	1.35	1.73

Two different planar cross sections through the reactor are distinguished by the addition of UC (upper core ≙ control rods partially inserted) and LC (lower core ≙ control rods replaced by sodium followers), respectively. Additionally two different core configurations are distinguished by a preceding N (normal core) or V (voided core).

To demonstrate the possible influence of discretization and rounding errors on the final results, the following illustrative sketch is used showing only systematic effects but it is characteristic for all calculated results.



k_{eff} as a function of mesh refinements (average area per mesh point) for the normal and voided core configuration and for the upper and lower core model, respectively.

The lines parallel to the x-axis show the k_{eff} values for the mesh size going to zero which is the idealized result attainable with diffusion calculations, free of discretization and rounding errors. The criticality differences y_{CRV}, y_{CRN}, y_{VL} and y_{VU} at the point x = 0 denote the idealized values for control rod worths and void reactivities. Of course it is not possible to obtain these results directly by reactor calculations. For each calculation we have to assume a mesh size of x_1, different from zero. For $x_1 \neq 0$ Δk_{DVU}, Δk_{DNU}, Δk_{DVL} and Δk_{DNL} denote the discretization and Δk_{RVL}, Δk_{RVU}, Δk_{RNL} and Δk_{RNU} the rounding errors for all cases under consideration.* (In the following the rounding error is assumed to be equivalent to the differences between the DIXY-IA and the DIXY-KfK values.)

From the sketch it can be seen easily that errors in k_{eff} usually also cause errors in control rod worths Δk_{CRV} and Δk_{CRN} and also in void reactivities Δk_{VL} and Δk_{VU} even for the DIXY-IA results.

$$\Delta k_{CRV} = y_{CRV} + \Delta k_{DVU} - \Delta k_{DVL}$$
$$\Delta k_{CRN} = y_{CRN} + \Delta k_{DNU} - \Delta k_{DNL}$$
$$\Delta k_{VL} = y_{VL} + \Delta k_{DNL} - \Delta k_{DVL}$$
$$\Delta k_{VU} = y_{VU} + \Delta k_{DNU} - \Delta k_{DVU}$$

Generally $\Delta k_{DVU} \neq \Delta k_{DVL}$, $\Delta k_{DNU} \neq \Delta k_{DNL}$, $\Delta k_{DNL} \neq \Delta k_{DVL}$ and $\Delta k_{DNU} \neq \Delta k_{DVU}$ because of the different gradients of the k_{eff} lines as a function of AAMP. In the case of DIXY-KfK calculations also rounding errors have to be taken into account:

$$\Delta k_{CRV} = y_{CRV} + \Delta k_{DVU} - \Delta k_{DVL} + \Delta k_{RVU} - \Delta k_{RVL}$$
$$\Delta k_{CRN} = y_{CRN} + \Delta k_{DNU} - \Delta k_{DNL} + \Delta k_{RNU} - \Delta k_{RNL}$$
$$\Delta k_{VL} = y_{VL} + \Delta k_{DNL} - \Delta k_{DVL} + \Delta k_{RNL} - \Delta k_{RVL}$$
$$\Delta k_{VU} = y_{VU} + \Delta k_{DNU} - \Delta k_{DVU} + \Delta k_{RNU} - \Delta k_{RVU}$$

Primarily, the existing criticality data for UC- and LC-models have been reanalyzed. The evaluation leads to a reasonable judgement of the uncertainties caused by discretization and rounding errors. After these intrinsic difficulties of the DIXY-KfK program became evident for k_{eff} and the

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* The sign of these errors has been defined in a convenient way so that most of them have a positive sign.

control rod worth, similar results for sodium void effects have been desired. For that purpose the benchmark calculations for the normal core (NUC, NLC) were repeated for a voided core (VUC, VLC) situation and the results were analyzed in the analogous manner.*)

A detailed understanding of the problem of discretization and rounding errors has been obtained, after all models have been recalculated by the DIXY-IA version on a Cyber 172 computer using an internal data representation of 60 bits per word. The values for k_{eff} are summarized in Table 1 for all models under consideration. The k_{eff} values for AAMP = 0 are determined as a reasonable linear extrapolation of the other values. They are considered to be fairly reliable but of course these values are subject to small uncertainties and, therefore, should not be taken as exact results. This fact should be taken into account if discretization errors for small mesh sizes are evaluated and if the extrapolation of the discretization error to infinitely small mesh size does not lead exactly to the expected value.

TABLE 1: VALUES OF KEFF OBTAINED BY DIXY-IA FOR NORMAL AND VOIDED CORES OF THE SNR-300 BENCHMARK, DEPENDENT ON DISCRETIZATION SCHEME.

AAMP	MODEL	NORMAL CORE	MODEL	VOIDED CORE
27.72	B1-NUC	1.104610	B1-VUC	1.126892
6.93	B2-NUC	1.108409	B2-VUC	1.130359
3.08	B3-NUC	1.109217	B3-VUC	1.131082
1.73	B4-NUC	1.109510	B4-VUC	1.131350
0.0		1.109878		1.131616
27.72	B1-NLC	1.245245	B1-VLC	1.272855
6.93	B2-NLC	1.246347	B2-VLC	1.274344
3.08	B3-NLC	1.246547	B3-VLC	1.274623
1.73	B4-NLC	1.246609	B4-VLC	1.274710
0.0		1.246710		1.274839

The corresponding values calculated by DIXY-KfK are summarized in Table 2. In this case linear extrapolated values for AAMP = 0 are of no practical meaning, they are replaced therefore by zeros.

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*) For all calculations a convergence criterion of $1 \cdot 10^{-4}$ was used.

TABLE 2: VALUES OF KEFF OBTAINED BY DIXY-KFK FOR NORMAL AND VOIDED CORES OF THE SNR-300 BENCHMARK, DEPENDENT ON DISCRETIZATION SCHEME.

AAMP	MODEL	NORMAL CORE	MODEL	VOIDED CORE
27.72	B1-NUC	1.104471	B1-VUC	1.126842
6.93	B2-NUC	1.108296	B2-VUC	1.130161
3.08	B3-NUC	1.108923	B3-VUC	1.130656
1.73	B4-NUC	1.108819	B4-VUC	1.130683
0.0		0.0		0.0
27.72	B1-NLC	1.245135	B1-VLC	1.272787
6.93	B2-NLC	1.246135	B2-VLC	1.274078
3.08	B3-NLC	1.246149	B3-VLC	1.274068
1.73	B4-NLC	1.245762	B4-VLC	1.273828
0.0		0.0		0.0

The values obtained by DIXY-IA can be considered to be essentially free of rounding errors. This assumption is of course somewhat too optimistic but at least the rounding errors are negligibly small for the purpose of the present study. This can be concluded from Figures 1 - 6*) which show the same linear behaviour for k_{eff} as a function of average area per mesh point for the DIXY-IA results as for all other codes in competition for the benchmark calculations /3,4/ and moreover the discrepances to the CITATION results are less than $5 \cdot 10^{-5}$ in going to mesh step → 0 although CITATION is a code using mesh centered discretization formulae (MCDF) whereas DIXY uses mesh edged discretization formulae (MEDF). A rounding error for these results which at maximum would amount to $5 \cdot 10^{-5}$ will not essentially change the conclusions obtained in this study. Following that argument, the differences between the DIXY-IA and the DIXY-KfK results will be taken as rounding errors. The following Tables 3 - 8 contain the important numerical results. Figs. 7 - 18 contain the corresponding information in graphical form.

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*) It should be mentioned that the ordinate scale in Figures 1 - 18 has been chosen such that the numerical values could be presented in an appropriate form. As a consequence, the scale is usually different between the various figures, even if similar quantities are considered (see e.g. Figs. 3 and 4).

Table 3 shows the discretization uncertainty concerning k_{eff}, calculated as

$$\Delta k_D(AAMP) = k_{eff_{IA}}(AAMP=0) - k_{eff_{IA}}(AAMP)$$

for the SNR-300 benchmark problem obtained by DIXY-IA, dependent on refinements of the mesh grid. The results are included in Figures 11 - 14 as functions denoted as discretization errors.

TABLE 3: KEFF DISCRETIZATION UNCERTAINTY FOR THE SNR 300 BENCHMARK OBTAINED BY DIXY-IA, DEPENDENT ON DISCRETIZATION SCHEME.

AAMP	NUC	NLC	VUC	VLC
27.72	0.52671E-02	0.14648E-02	0.47235E-02	0.19846E-02
6.93	0.14687E-02	0.36240E-03	0.12569E-02	0.49496E-03
3.08	0.66090E-03	0.16308E-03	0.53406E-03	0.21648E-03
1.73	0.36716E-03	0.10109E-03	0.26608E-03	0.12970E-03

In Table 4 control rod worths dependent on mesh refinements are summarized for the normal and the voided core, respectively, calculated by DIXY-IA as differences of k_{eff} values for LC and UC models respectively. The results are included in Figures 7 and 8 together with the values obtained by DIXY-KfK. The discretization errors, calculated as differences of control rod worths

$$\text{DISCR ERR} = \Delta k_{CR}(AAMP \to 0) - \Delta k_{CR}(AAMP)$$

and the relative errors obtained by dividing these differences by $\Delta k_{CR}(AAMP)$ are also included in Table 4.

TABLE 4: CONTROL ROD WORTHS AND CORRESPONDING DISCRETIZATION UNCERTAINTIES OBTAINED FROM DIXY-IA RESULTS, DEPENDENT ON DISCRETIZATION SCHEME.

AAMP	NORMAL CORE			VOIDED CORE		
	DKEFF CR	DISCR ERR	REL.ERROR	DKEFF CR	DISCR ERR	REL.ERROR
27.72	0.141E+00	0.380E-02	0.270E-01	0.146E+00	0.274E-02	0.188E-01
6.93	0.138E+00	0.111E-02	0.802E-02	0.144E+00	0.762E-03	0.529E-02
3.08	0.137E+00	0.498E-03	0.362E-02	0.144E+00	0.318E-03	0.221E-02
1.73	0.137E+00	0.266E-03	0.194E-02	0.143E+00	0.136E-03	0.951E-03
0.0	0.137E+00	0.0	0.0	0.143E+00	0.0	0.0

Table 5 shows corresponding values for sodium void reactivities dependent on mesh refinements for the upper (UC) and the lower (LC) core, respectively, calculated as differences of k_{eff} values for the voided and the unvoided core

$$\Delta k_{VU}(AAMP) = k_{eff_{VUC}}(AAMP) - k_{eff_{NUC}}(AAMP)$$

$$\Delta k_{VL}(AAMP) = k_{eff_{VLC}}(AAMP) - k_{eff_{NLC}}(AAMP)$$

The results can be found in Figures 9 and 10 together with the values obtained by DIXY-KfK. Discretization errors and relative errors are also included in this table in the same way as done for Table 4.

TABLE 5: SODIUM VOID REACTIVITY VALUES AND CORRESPONDING DISCRETIZATION UNCERTAINTIES OBTAINED FROM DIXY-IA RESULTS, DEPENDENT ON DISCRETIZATION SCHEME.

AAMP	UC (ABSORBERS PART. INSERTED)			LC (ABSORB. REPL. BY FOLLOWERS)		
	DKEFF(VD)	DISCR ERR	REL.ERROR	DKEFF(VD)	DISCR ERR	REL.ERROR
27.72	0.223E-01	0.544E-03	0.244E-01	0.276E-01	-0.520E-03	-0.188E-01
6.93	0.219E-01	0.212E-03	0.965E-02	0.280E-01	-0.133E-03	-0.473E-02
3.08	0.219E-01	0.127E-03	0.580E-02	0.281E-01	-0.534E-04	-0.190E-02
1.73	0.218E-01	0.101E-03	0.463E-02	0.281E-01	-0.286E-04	-0.102E-02
0.0	0.217E-01	0.0	0.0	0.281E-01	0.0	0.0

In Table 6 results obtained by DIXY-KfK are compared with those calculated by DIXY-IA. Besides the discretization error Δk_D of Table 3 the rounding errors calculated as differences of k_{eff} values

$$\Delta k_R(AAMP) = k_{eff}(DIXY\text{-}IA, AAMP) - k_{eff}(DIXY\text{-}KfK, AAMP)$$

and the total errors obtained as differences of

$$\Delta k_T(AAMP) = k_{eff}(DIXY\text{-}IA, AAMP{=}0) - k_{eff}(DIXY\text{-}KfK, AAMP)$$

are summarized in Table 6 dependent on mesh refinements for all core configurations NUC, NLC, VUC and VLC.

TABLE 6: COMPARISON OF DISCRETIZATION, ROUNDING (DKEFFR=KEFF(DIXY-IA)-KEFF(DIXY-KFK)) AND TOTAL ERRORS (DKEFFT=DISCR.+ROUND. ERRORS=KEFF(DIXY-IA,AAMP=0)-KEFF(DIXY-KFK)), DEPENDENT ON THE DISCRETIZATION SCHEME.

AAMP	NUC			NLC		
	DKEFFD	DKEFFR	DKEFFT	DKEFFD	DKEFFR	DKEFFT
27.72	0.52671E-02	0.13924E-03	0.54064E-02	0.14648E-02	0.10967E-03	0.15745E-02
6.93	0.14687E-02	0.11253E-03	0.15812E-02	0.36240E-03	0.21267E-03	0.57507E-03
3.08	0.66090E-03	0.29373E-03	0.95463E-03	0.16308E-03	0.39768E-03	0.56076E-03
1.73	0.36716E-03	0.69141E-03	0.10586E-02	0.10109E-03	0.84686E-03	0.94795E-03

AAMP	VUC			VLC		
	DKEFFD	DKEFFR	DKEFFT	DKEFFD	DKEFFR	DKEFFT
27.72	0.47235E-02	0.50545E-04	0.47741E-02	0.19846E-02	0.67711E-04	0.20523E-02
6.93	0.12569E-02	0.19741E-03	0.14544E-02	0.49496E-03	0.26608E-03	0.76103E-03
3.08	0.53406E-03	0.42534E-03	0.95940E-03	0.21648E-03	0.55504E-03	0.77152E-03
1.73	0.26608E-03	0.66662E-03	0.93269E-03	0.12970E-03	0.88215E-03	0.10118E-02

Table 7 shows in addition to the original values for the control rod reactivities and the associated discretization errors of Table 4 the corresponding rounding and total errors as well as the relative uncertainties for the normal and voided core, respectively. Corresponding graphs are given in Figs. 7, 8, 15 and 16. The quantities are calculated according to the following definitions:

$$\Delta k_{RN}(CR) = \Delta k_R(NUC) - \Delta k_R(NLC)$$

$$\Delta k_{RV}(CR) = \Delta k_R(VUC) - \Delta k_R(VLC)$$

$$\Delta k_{TN}(CR) = \Delta k_{DN}(CR) + \Delta k_{RN}(CR) = k_{eff}\left[\text{DIXY-IA(NUC,AAMP}\rightarrow 0\right] - k_{eff}\left[\text{DIXY-KfK(NUC,AAMP)}\right] - \left[k_{eff}\left[\text{DIXY-IA(NLC,AAMP}\rightarrow 0\right] - k_{eff}\left[\text{DIXY-KfK(NLC,AAMP)}\right]\right]$$

$$\Delta k_{TV}(CR) = \Delta k_{DV}(CR) + \Delta k_{RV}(CR) = k_{eff}\left[\text{DIXY-IA(VUC,AAMP}\rightarrow 0\right] - k_{eff}\left[\text{DIXY-KfK(VUC,AAMP)}\right] - \left[k_{eff}\left[\text{DIXY-IA(VLC,AAMP}\rightarrow 0\right] - k_{eff}\left[\text{DIXY-KfK(VLC,AAMP)}\right]\right]$$

$\Delta k_R(NUC)$, $\Delta k_R(NLC)$, $\Delta k_R(VUC)$ and $\Delta k_R(VLC)$ used from Table 6, k_{eff} values coming from Table 1 and Table 2, respectively.

TABLE 7: COMPARISON OF DISCRETIZATION AND ROUNDING ERRORS AND THE CORRESPONDING TOTAL AND RELATIVE NUMERICAL UNCERTAINTIES FOR THE CONTROL ROD WORTHS.

AAMP	NORMAL CORE				
	DKEFF CR	DISCR ERR	DKEF(CR)R	DKEF(CR)T	REL.ERROR
27.72	0.141E+00	0.380E-02	0.296E-04	0.383E-02	0.272E-01
6.93	0.138E+00	0.111E-02	-0.100E-03	0.101E-02	0.729E-02
3.08	0.137E+00	0.498E-03	-0.104E-03	0.394E-03	0.287E-02
1.73	0.137E+00	0.266E-03	-0.155E-03	0.111E-03	0.807E-03

AAMP	VOIDED CORE				
	DKEFF CR	DISCR ERR	DKEF(CR)R	DKEF(CR)T	REL.ERROR
27.72	0.146E+00	0.274E-02	-0.172E-04	0.272E-02	0.186E-01
6.93	0.144E+00	0.762E-03	-0.687E-04	0.693E-03	0.482E-02
3.08	0.144E+00	0.318E-03	-0.130E-03	0.188E-03	0.131E-02
1.73	0.143E+00	0.136E-03	-0.216E-03	-0.792E-04	-0.552E-03

Besides the sodium void reactivity values and the corresponding discretization uncertainties of Table 5 the rounding and the total errors as well as the relative numerical uncertainties for the sodium void reactivity are summarized in Table 8 for the lower and the upper core, respectively. Corresponding graphs are shown in Figs. 9, 10, 17 and 18. The definitions are as follows:

$$\Delta k_{RL}(VOID) = \Delta k_R(VLC) - \Delta k_R(NLC)$$

$$\Delta k_{RU}(VOID) = \Delta k_R(VUC) - \Delta k_R(NUC)$$

$$\Delta k_{TL}(VOID) = \Delta k_{DL}(VOID) + \Delta k_{RL}(VOID) = k_{eff}[DIXY\text{-}IA(VLC,AAMP\rightarrow O)]$$
$$-k_{eff}[DIXY\text{-}KfK(VLC,AAMP)] - \left[k_{eff}[DIXY\text{-}IA(NLC,AAMP\rightarrow O)] - k_{eff}[DIXY\text{-}KfK(NLC,AAMP)]\right]$$

$$\Delta k_{TU}(VOID) = \Delta k_{DU}(VOID) + \Delta k_{RU}(VOID) = k_{eff}[DIXY\text{-}IA(VUC,AAMP\rightarrow O)]$$
$$-k_{eff}[DIXY\text{-}KfK(VUC,AAMP)] - \left[k_{eff}[DIXY\text{-}IA(NUC,AAMP\rightarrow O)] - k_{eff}[DIXY\text{-}KfK(NUC,AAMP)]\right]$$

using $\Delta k_R(VLC)$, $\Delta k_R(NLC)$, $\Delta k_R(VUC)$ and $\Delta k_R(NUC)$ from Table 6 and k_{eff} values from Table 1 and 2, respectively.

TABLE 8: COMPARISON OF DISCRETIZATION AND ROUNDING ERRORS AND THE CORRESPONDING TOTAL AND RELATIVE NUMERICAL UNCERTAINTIES FOR THE NA-VOID REACTIVITY.

AAMP	LOWER CORE				
	DKEFF VD	DISCR ERR	DKEF(VD)R	DKEF(VD)T	REL.ERR
27.72	0.276E-01	-0.520E-03	0.420E-04	-0.478E-03	-0.214E-01
6.93	0.280E-01	-0.133E-03	-0.534E-04	-0.186E-03	-0.847E-02
3.08	0.281E-01	-0.534E-04	-0.157E-03	-0.211E-03	-0.964E-02
1.73	0.281E-01	-0.286E-04	-0.353E-04	-0.639E-04	-0.293E-02

AAMP	UPPER CORE				
	DKEFF VD	DISCR ERR	DKEF(VD)R	DKEF(VD)T	REL.ERR
27.72	0.223E-01	0.544E-03	0.887E-04	0.632E-03	0.229E-01
6.93	0.219E-01	0.212E-03	-0.849E-04	0.127E-03	0.453E-02
3.08	0.219E-01	0.127E-03	-0.132E-03	-0.477E-05	-0.170E-03
1.73	0.218E-01	0.101E-03	0.248E-04	0.126E-03	0.448E-02

IV Discussion of the Results for the SNR-300 Benchmark Calculations

a) Discretization Uncertainty

The results presented in Table 3 and Figs. 3 - 6 or Figs. 11 - 14, respectively, demonstrate that the discretization uncertainty depends on the configuration studied. From Tables 3 and 6 it can be deduced that discretization uncertainties smaller than $1 \cdot 10^{-3}$ and $1 \cdot 10^{-4}$, respectively, can be obtained if the following rough values for AAMP* are not exceeded:

	Maximum allowable AAMP [cm^2]			
k_{eff}-discret. uncertainty	NUC	NLC	VUC	VLC
$1 \cdot 10^{-3}$	4.7	19.	5.5	14.0
$1 \cdot 10^{-4}$	0.47	1.9	0.55	1.4

The criticality difference shown in Figs. 7 and 8 between k_{eff}(UC) and k_{eff}(LC) is considered to be representative of the reactivity effect of a large amount of absorber. From Tables 4 and 7 and the corresponding Figs. 15 and 16 we conclude that the following AAMP-values should not be exceeded in order to keep DISCR ERR (CR) the absolute discretization error for $\Delta k_{eff,CR}$ = DKEFF CR below $1 \cdot 10^{-3}$ and $1 \cdot 10^{-4}$, respectively.

	Maximum allowable AAMP [cm^2]	
DISCR ERR (CR)	NC	VC
$1 \cdot 10^{-3}$	6.3	7.5
$1 \cdot 10^{-4}$	0.6	$\sim$ 0.7**

* The corresponding mesh sizes can be roughly determined as the square root of the values for AAMP.

** As mentioned before, the extrapolation of the discretization uncertainties for k_{eff} is subject to small uncertainties; hence, the extrapolation of discretization uncertainties for Δk-values is usually even more unreliable since the difference of extrapolated k_{eff}-discretization uncertainties is involved.

In a similar way as before, the criticality difference shown in Figs. 9 and 10 between k_{eff}(VC) and k_{eff}(NC) is considered to be typical for the whole core sodium void effect. Tables 5 and 8 and the corresponding Figs. 17 and 18 for the upper core (poisoned core) and the lower core (normal core) lead to the conclusion that the following AAMP-values should not be exceeded in order to keep DISCR ERR (VD), the absolute discretization error for $\Delta k_{eff,VD}$ = DKEFF VD, below $1 \cdot 10^{-3}$ and $1 \cdot 10^{-4}$, respectively.

	Maximum allowable AAMP [cm^2]	
DISCR ERR (VD)	PC ≙ UC	NC ≙ LC
$1 \cdot 10^{-3}$	∿ 40.	∿ 53
$1 \cdot 10^{-4}$	∿ 1.7*	5.3

b) Rounding Errors

It is evident from Table 6 that it is impossible to keep the rounding error smaller than $1 \cdot 10^{-4}$ when using present DIXY-version at KfK. Unfortunately but quite naturally, the rounding error generally increases with decreasing mesh size and decreasing AAMP-values; i.e. the tendency is just opposite to the discretization uncertainty. From Figs. 11 - 14 it can be deduced that both quantities have about equal amounts at the following AAMP-values

AAMP-values [cm^2] at which DKEFFD ≃ DKEFFR ≃ 1/2 DKEFFT

NUC		NLC		VUC		VLC	
1/2 DKEFFT	AAMP	1/2 DKEFFT	AAMP	1/2 DKEFFT	AAMP	1/2 DKEFFT	AAMP
$5 \cdot 10^{-4}$	2.3	$3 \cdot 10^{-4}$	5.5	$4.5 \cdot 10^{-4}$	2.8	$4.0 \cdot 10^{-4}$	5.0

It goes without saying that a certain numerical error of the k_{eff}-results obtained with DIXY-KfK has to be tolerated. These minimum total k_{eff}-uncertainties are deduced in a rough manner from Figs. 11 - 14. They are

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* see footnote for the preceding table.

given in the following tabulation together with the corresponding approximate AAMP-values for which these minimum uncertainties can be attained.

Minimum total k_{eff}-uncertainties DKMT with DIXY-KfK and corresponding AAMP-values [cm^2]

NUC		NLC		VUC		VLC	
DKMT	AAMP	DKMT	AAMP	DKMT	AAMP	DKMT	AAMP
$1 \cdot 10^{-3}$	3.0	$5 \cdot 10^{-4}$	5.0	$9 \cdot 10^{-4}$	2.5	$7 \cdot 10^{-4}$	4.0

Figs. 15 - 18 for the criticality differences DKEFF CR and DKEFF VD demonstrate that in many cases a partial cancellation occurs between the discretization uncertainty and the rounding error which may have a sign opposite to that of the discretization uncertainty. But this fact may be fortuitous and specific for the present example. At least the amount of mutual cancellation will most probably be different if a different reactor design has to be analyzed. Since in most of the cores studied the influence of the rounding error on the void reactivities and especially on the control rod reactivities is usually not too pronounced, compared to the importance of the discretization uncertainty, it might be sufficient for most purposes or at least be a reasonable suggestion for further applications to use as a safe estimate the preceding values based solely on the discretization uncertainty as an approximate basis for a meaningful guess of the numerical accuracy of both reactivities as a function of mesh size or AAMP.

The calculated control rod reactivity is fairly large in the present example. Therefore, numerical effects of the order of $1 \cdot 10^{-4}$ or lower may not become evident. On the other hand one should not conclude from Figs. 15 and 16 of the present study, that in all cases the absorber reactivity can be obtained with sufficient accuracy. The difficulties discussed before for k_{eff} and mentioned in the following for the sodium void reactivity suggest that it might be difficult to determine reactivity effects which are appreciably smaller than some 10^{-4} with acceptable reliability using the present DIXY-KfK version. It seems to be more prudent to cast some doubts on all reactivity values of that magnitude which have been determined by successive criticality calculations using this version of the code.

V General Aspects Derived from the Benchmark Results

From Figs. 17 and 18 it can be expected that it might be difficult to determine the whole core sodium void reactivity with an accuracy better than roughly $1 \cdot 10^{-4}$ using DIXY-KfK. Although an uncertainty of about that amount seems to be tolerable for the present case and probably also for a lot of other practical purposes, one should have in mind that for other reactivity effects this uncertainty of about $1 \cdot 10^{-4}$ may also represent a principal lower limit for the accuracy attainable with the present version of DIXY-KfK. If that conjecture would turn out to be valid generally, i.e. if it is some kind of an intrinsic feature of reactivity values deduced from k_{eff}-results obtained by DIXY-KfK this might in some specific cases severely influence the kind of analysis of small reactivity values. Such small reactivity effects (which can be attributed either to a small perturbed region or - even worse - to a small net effect for a fairly extended perturbed region produced by cancellation of fairly large contributions of different signs) should then no longer be determined by successive criticality calculations. Using the equivalence $1\ \$ \approx 0.004\ \Delta k$ it can be supposed that the evaluation of reactivity effects becomes doubtful if effects of the order of 50 ¢ or lower are analyzed by that method. For these purposes the application of exact or sometimes first order perturbation theory is probably more appropriate.

With respect to the results of Ganesan /1/ it is important to note that the limit found above for the accuracy of the whole core sodium void reactivity by far exceeds the crucial quantity of $\delta(\Delta k_{Void}) \approx 1.3 \cdot 10^{-5}$*) which

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*) With respect to such a small magnitude for a deviation between corresponding reactivity values the following remark might be adequate to illustrate the assumptions frequently made in evaluating nuclear reactor calculations made with DIXY. It has been observed frequently that the converged k_{eff}-values and especially the criticality differences have a remarkably better convergence accuracy than that given by the limiting values printed in the DIXY output listing as upper and lower k_{eff}-boundaries. Assuming the general validity of this experience, it seemed to be justified to bother about a discrepancy of the order of $1.3 \cdot 10^{-5}$ although it is admitted in /1/ that this value is smaller than the convergence criterion which could be applied using a reasonable amount of computer time. For the same reason it was somewhat surprising that the discrepancy could not be eliminated or at least substantially mitigated by refining the mesh size or by requiring a stronger convergence criterion.

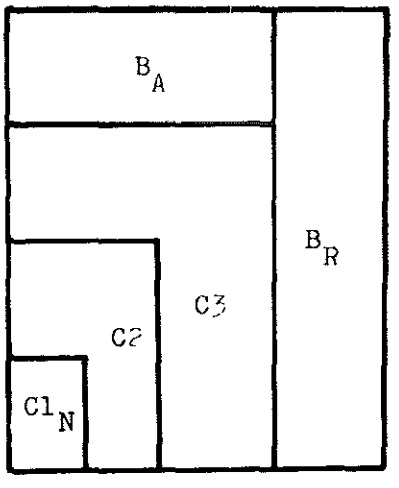
was responsible for the confusion about the puzzling disagreement between the results of the criticality difference obtained from direct criticality calculations and the corresponding exact perturbation theory results. Even if one takes into account that in the case studied by Ganesan /1/ only a restricted volume of the core region has been voided, and, in addition, an r-z-geometry has been treated, the preceding study indicates that one should also in this case be cautious upon relying on small reactivities determined by successive criticality calculations. According to our present experience it seems in our opinion to be advisable to consider these results as fairly dubious.

According to the experience gained for the SNR-300-Benchmark it was obvious that some reevaluation of the Ganesan work /1/ might now reveal the proper reasons for the difficulties encountered previously in /1/. This reevaluation would also add some knowledge with respect to results for r-z-geometry (the benchmark results apply to x-y-geometry). As mentioned before the number of energy groups has been reduced to 4. This yields a tremendous reduction in computing time but, of course, leads to deviations with respect to the numerical result for the sodium void effect which has originally been derived in /1/ using 26 energy groups. It is expected that the main reasons for the difficulties observed in /1/ are essentially independent of the number of energy groups. The new results for the Ganesan-case are discussed in the next chapter.

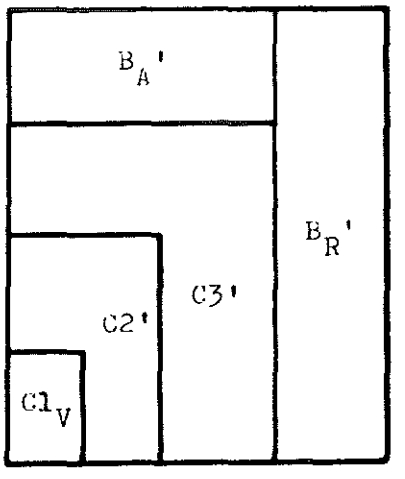
VI Results of 4-Group Studies for the GANESAN-Case A-Configuration

For these studies two series of calculations have been performed. The following sketches should help to explain the peculiarities for the different series of calculations.

a) Sketch 1 and 2 show schematically the normal and the central voided core configurations, respectively. For the first series two different

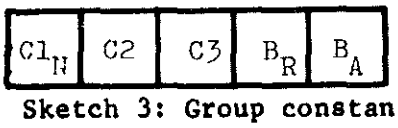


Sketch 1: Normal core configuration

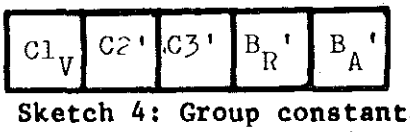


Sketch 2: Central voided core configuration

data sets of 4 energy group constants have been established as shown in sketches 3 and 4.



Sketch 3: Group constants for normal core configuration

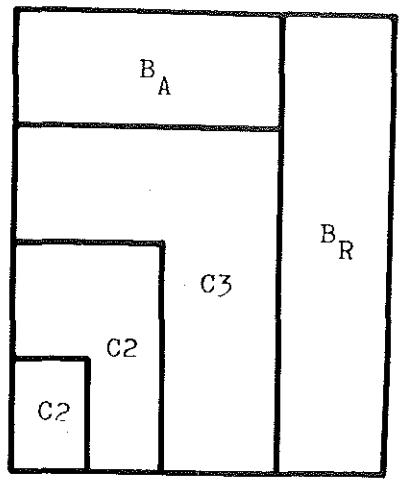


Sketch 4: Group constants for central voided core configuration

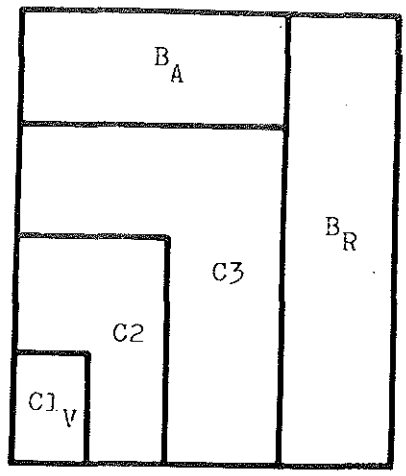
Two different 1-dimensional models for the corresponding core configurations have been used for generating the appropriate condensation spectra. For this reason not only the group constants for the unvoided $C1_N$ and the central voided $C1_V$ core regions are different but also C2 ≠ C2', C3 ≠ C3' ..., although the material compositions are identical. One has to keep in mind that for an equivalent reason also the group constants for $C1_N$ and C2 are slightly different although their material compositions are exactly the same.

b) For the second series a somewhat different procedure has been chosen, leading to a simpler calculational model. Only one single 4 group constant

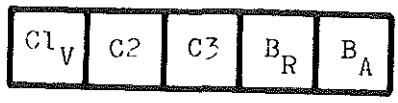
data set was established using the 4 group constant sets already mentioned in sketches 3 and 4. The core configurations are shown in the sketches 5 and 6 and the combined group constant set is given in sketch 7.



Sketch 5: Normal core configuration



Sketch 6: Central voided core configuration



Sketch 7: Group constants for normal and central voided core configuration

Exact perturbation calculations for the void reactivity are obviously facilitated when using the simpler model b) which might be a somewhat poorer approximation from the neutronics point of view but still provides a firm basis for numerical intercomparisons from the mathematical point of view, whereas procedure a) aims at a more correct representation of the neutronic aspects.

The corresponding results for the criticality and reactivity values are very similar for these two different series of calculations, a) and b), respectively. Therefore it seems sufficient for the present purpose to show and discuss only the results of procedure b) in connection with corresponding results of exact perturbation calculations. Other calculations done parallel to the present study led to the suspicion that possibly the results of the direct and adjoint cases do not agree within the accuracy limits specified as input to the diffusion program. This fact has then been

verified for the present case too as is illustrated by the following examples showing the DIXY-KfK-results for the mesh grid 96*112. The upper and lower k_{eff}-boundaries Q_{max} and Q_{min}, respectively, are also taken from the DIXY-output.

Case	Configuration					
	Normal			Voided		
	Q_{min}	k_{eff}	Q_{max}	Q_{min}	k_{eff}	Q_{max}
Direct	0.9945772	0.9945966	0.9946005	0.9947796	0.9947885	0.9947903
Adjoint	0.9946545	0.9946684	0.9946704	0.9948494	0.9948629	0.9948661

Therefore, in the following Tables 9 and 10 all criticality values and all corresponding reactivities derived from them are given.

The results for $k^{+}_{eff\ N}$ and $k_{eff\ V}$ are shown in Fig. 19 as a function of the average area per meshpoint in the core region $\overline{AAMP}_c = (R_c \cdot H_c/2)/P_{rc} \cdot P_{zc}$, where R_c = core radius ≈ 36 cm, $H_c/2$ = half core height of the symmetric reactor ≈ 31 cm, P_{rc} = radial meshpoints in the core region, P_{zc} = axial mesh points in the core region.

Table 9: Criticality Values for the Ganesan - Case A - Configuration

Mesh-Grid*)	DIXY Source Accuracy**)	Configuration			
		Normal		Voided	
		k_{effN}	k^{+}_{effN}	k_{effV}	k^{+}_{effV}
12*14	$1 \cdot 10^{-4}$	0.9903294	0.9903293	0.9905149	0.9905149
24*28	"	0.9949550	0.9949564	0.9951394	0.9951394
48*56	$5 \cdot 10^{-5}$	0.9957617	0.9957466	0.9959455	0.9959312
96*112	$2 \cdot 10^{-5}$	0.9945966	0.9946684	0.9947885	0.9948629

k_{eff} ≙ criticality for direct problem

k^{+}_{eff} ≙ criticality for adjoint problem

*) Here the total number of mesh points is given. For the first case 8 mesh points in radial and 7 mesh points in the axial direction have been used in the core region. Upon mesh refinements the number of mesh points in the core region has always been doubled for each direction.

**) The criterion for the relative accuracy of the fluxes in all cases amounted to five times the values given for the source accuracy.

Table 10: Criticality Differences for the Ganesan - Case A - Configuration

Mesh Grid	Average Core Mesh Sizes		Exact Perturbation Calculation * 10^4 *)	$(k_{effV} - k_{effN}) \cdot 10^4$	$(k^+_{effV} - k^+_{effN}) \cdot 10^4$	$(k_{effV} - k^+_{effN}) \cdot 10^4$	$(k^+_{effV} - k_{effN}) \cdot 10^4$
	h_r [cm]	h_z [cm]					
12*14	5.17	5.18	1.836	1.855	1.856	1.856	1.855
24*28	2.58	2.59	1.835	1.844	1.830	1.830	1.844
48*56	1.29	1.30	1.862	1.838	1.846	1.989	1.695
96*112	0.65	0.65	1.859	1.919	1.945	1.201	2.663

*) The values given are those printed as $\Delta k/k$-result in the DIXY output. Therefore it might have been more appropriate to compare them with eigenvalue differences, i.e. $|\Delta\lambda_V| = |(1/k_{effN}) - (1/k_{effV})|$. Furthermore, a really exact perturbation calculation was not possible with DXPERT at the time of performing the present study because the fission term is multiplied by the wrong eigenvalue. Both aspects are negligible for the present purpose. The actual values are averages of two results, one based on $(\phi^+_N, \delta\Sigma, \phi_V)$ and the other on $(\phi^+_V, \delta\Sigma, \phi_N)$. Both results agree with each other in the first three figures.

Before discussing the results of the preceding tables in detail, it should be mentioned that the absolute value of the void reactivity of about $1.8 \cdot 10^{-4}$ determined in our DIXY-KfK calculations for the Ganesan - Case A configuration is fairly small and is quite different from Ganesan's value /1/ of about $7 \cdot 10^{-5}$. The reason for this difference is most probably due to the different number of energy groups; Ganesan used 26 groups whereas here, as mentioned before, a collapsing to 4 groups has been done in advance to the diffusion calculations.

A comparison of the void reactivities given in Table 10 shows that the results of exact perturbation calculations are very reliable and nearly independent of the mesh grid used.

For mesh sizes exceeding roughly 2 cm in the core region one can observe a sufficiently close agreement between all Δk_{Void}-values determined in the different ways indicated in Table 10, at least if one disregards for the moment the possible influence of the discretization uncertainty which seems to be fairly small in this case.

The reactivities deduced from successive criticality calculations of the same kind, i.e. either direct $(k_{effV} - k_{effN})$ or adjoint $(k^{+}_{effV} - k^{+}_{effN})$ are also fairly reliable. Most probably this is an intrinsic feature of DIXY-KfK which may be due to a rather complete cancellation of rounding errors. If the mesh size is reduced below about 1 cm, the reliability of these above Δk-values worsens slightly but in our case the deviations do not exceed $1 \cdot 10^{-5}$. This amount is not really significant compared to the DIXY source accuracy amounting to at least $2 \cdot 10^{-5}$.

Void reactivities Δk_{Void} determined from cross differences of successive criticality calculations, i.e. $(k^{+}_{effV} - k_{effN})$ or $(k_{effV} - k^{+}_{effN})$ become somewhat unreliable if the mesh size is reduced below about 1.5 cm. The main reason is probably caused by deviations between direct and adjoint eigenvalues for the identical problem. These deviations may originate from the fact that rounding errors of the single precision DIXY-KfK version can have a different influence on the direct and the adjoint calculations and the corresponding eigenvalue of the solution obtained. In our case deviations up to about $7 \cdot 10^{-5}$ have been observed for $(k^{+}_{effV} - k_{effV})$ and $(k^{+}_{effN} - k_{effN})$ (see Table 9). These deviations directly propagate to the

Δk_{Void}-values just mentioned above.

Since Ganesan used in his study /1/ the difference ($k_{effV} - k^{+}_{effN}$) and a basic mesh grid of 40*50 mesh points for the whole reactor it is quite obvious from the results presented above, that his results could be effected by rounding errors of the order of $1 \cdot 10^{-5}$. Thus having in mind the results of the present work, it is no longer surprising that in Ganesan's work a rounding error could be responsible for the crucial quantity of $1.3 \cdot 10^{-5}$ which is representative for the somewhat puzzling discrepancy observed in /1/ between the results of perturbation calculations and the difference of criticality calculations for k_{effV} and k^{+}_{effN}. According to the present knowledge it seems to be inevitable that this situation could not be improved essentially upon a mesh refinement as Ganesan tried /1/. Quite on the contrary, such a procedure may even deteriorate the results as has been found in the present study.

From Table 9 and Fig. 19 it is evident that the results of the Ganesan - Case A calculations follow the same tendency as observed for the results of the preceding SNR-300 benchmark cases: a reduction of the mesh size does not necessarily lead to an improvement in accuracy and reliability of the calculated criticality value but, on the contrary, the effect of the rounding errors may become as large as $2 \cdot 10^{-3}$ Δk if fairly small mesh intervals of about 0.6 cm are used. In units of characteristic quantities for diffusion theory codes a mesh size of 0.6 cm is - in the important energy region relevant for fast reactors - roughly equivalent to 0.3 of the minimum transport mean free path or 0.1 of the minimum diffusion length. For the sake of completeness it should be mentioned that the finest mesh grid corresponded to a total number of spatial mesh points of about 10,000.

VII Summary and Conclusions

The results of the present study can be summarized as follows:

1. The inconsistencies of the DIXY-KfK results for the benchmark problem as well as for the Ganesan problem which have been observed previously for small mesh steps have their origin in the single precision of internal data representation of this version on the IBM 370/168 available at KfK.*

2. The discretization error depends approximately in a linear way on AAMP, the average area per mesh point.

3. Mesh refinements do not necessarily lead to an improved accuracy of DIXY-KfK k_{eff}-values because the according reduction of the discretization error may be more than counterbalanced by an increased contribution of the rounding error to the total k_{eff}-uncertainty.

4. The comparison of DIXY-KfK and DIXY-IA results leads to values of the optimum accuracy which can be attained for the benchmark configuration upon application of DIXY-KfK. The fact that no better accuracies can presently be reached is due to the combined influence of discretization and rounding errors existing with the single precision version of DIXY-KfK (e.g. Figure 14).

5. For mesh interval values exceeding roughly 2 cm in the core region one can observe a sufficiently close agreement between the various reactivity values determined in different ways.

6. The results of direct and adjoint calculations for the same configuration do not always agree within the accuracy limits specified as input requirements to the diffusion program. In our study a maximum deviation of about $7 \cdot 10^{-5}$ has been observed for a case of about 10,000 mesh points corresponding to a mesh interval size of about 0.6 cm.

   This leads to the following perceptions:

   a) Reactivities deduced from successive criticality differences for

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* Work on a DIXY-version with double precision is in progress at KfK.

either direct (real) or adjoint problems, i.e. (k_{eff}(perturbed) - k_{eff}(unperturbed)) or (k^+_{eff}(perturbed) - k^+_{eff}(unperturbed)) are fairly reliable. In our case the most pronounced deviation occurred at a mesh size of roughly 0.6 cm and amounted to about $1 \cdot 10^{-5}$ which is smaller than accuracy really obtained with the diffusion calculation.

b) As one could expect from the preceding comments, the cross differences of successive criticality calculations combining real and adjoint cases, i.e. (k_{eff}(perturbed) - k^+_{eff}(unperturbed)) or (k^+_{eff}(perturbed) - k_{eff}(unperturbed)) lead to somewhat unreliable criticality values if the mesh size is reduced below about 1.5 cm. In correspondence to comment 6, a maximum absolute deviation of about $7 \cdot 10^{-5}$ compared to the correct value has been found in the present study. This amount by far exceeds the crucial quantity of about $1.3 \cdot 10^{-5}$ which was responsible for the puzzling disagreement observed by Ganesan /1/ between the results of the criticality difference ($k_{eff\ void}$ - $k^+_{eff\ normal}$) and the corresponding exact perturbation theory result.

7. The results of exact perturbation calculations turned out to be very reliable in all cases especially when a refinement of the mesh grid may lead to unreliable criticality differences from successive criticality calculations.
   [The validity and importance of this statement is probably related to or influenced by
   a) the presence of rounding errors
   b) the limitation of the accuracy normally attainable within acceptable computing time during the usual iteration process in multidimensional diffusion programs.]

From our results the following recommendations can be deduced:

8. A DIXY version using double precision for the internal data representation on the IBM 370/168 is highly desirable at KfK.

9. If small reactivity values of the order of or less than about 1 $ ≈ 0.004 Δk have to be calculated the application of exact perturbation theory is highly preferable to the use of differences between successive criticality calculations. This comment applies to the numerical reliability and to the amount of computing time which has to be spent in order to attain a certain accuracy.

10. Using the single precision DIXY-KfK version the total k_{eff}-uncertainty (including discretization and rounding errors) can hardly be reduced below about $5 \cdot 10^{-4}$. Therefore, it seems more advisable to consider $1 \cdot 10^{-3}$ as a more realistic guess of the optimum accuracy which can presently be obtained with DIXY-KfK. These best accuracies can be obtained for mesh sizes between 1.5 and 2.5 cm. Both a reduction and an increase of the mesh size from the optimum value cause a deterioration of the attainable k_{eff}-accuracy.

11. If only the discretization error has to be taken into account, i.e. for the case of the DIXY-IA results or for future results obtained with the desired double precision DIXY-KfK version, the following somewhat rough AAMP-values should not be exceeded.

Maximum allowable AAMP-values [cm^2] for k_{eff}, whole core poison reactivity and whole core void reactivity (These rough values should not be exceeded in order to keep the discretization error below the uncertainty limits of $1 \cdot 10^{-3}$ and $1 \cdot 10^{-4}$, respectively.)

	Desired Quantity			
Uncertainty	k_{eff} Normal Core	k_{eff} Poisoned Core	Δk_{poison}	Δk_{void}
	AAMP	AAMP	AAMP	AAMP
$1 \cdot 10^{-3}$	20.	6.0	8.0	50.
$1 \cdot 10^{-4}$	2.	0.6	0.8	5.

As a concluding remark it should be mentioned that the present investigations refer solely to two specific cases: the 4 group SNR-300 benchmark in x-y-geometry and the 4 group SNEAK 9C2-critical in r-z-geometry. Therefore, the results, conclusions and recommendations derived here should be applied primarily to reactor configurations similar to those studied here. For reactors which are quite different from those of the present study or for other quantities to be determined which are not considered in this study, e.g. the reactivity worth of a single absorber

rod, the present work can only provide some limits about the probable magnitude of calculational uncertainties. Therefore, the experience deduced from our investigations should not be transferred directly to completely different situations but should then be taken only as a certain guideline which indicates that one should be fairly cautious upon the numerical accuracy and reliability of criticality - and reactivity - values determined with the present DIXY-KfK version.

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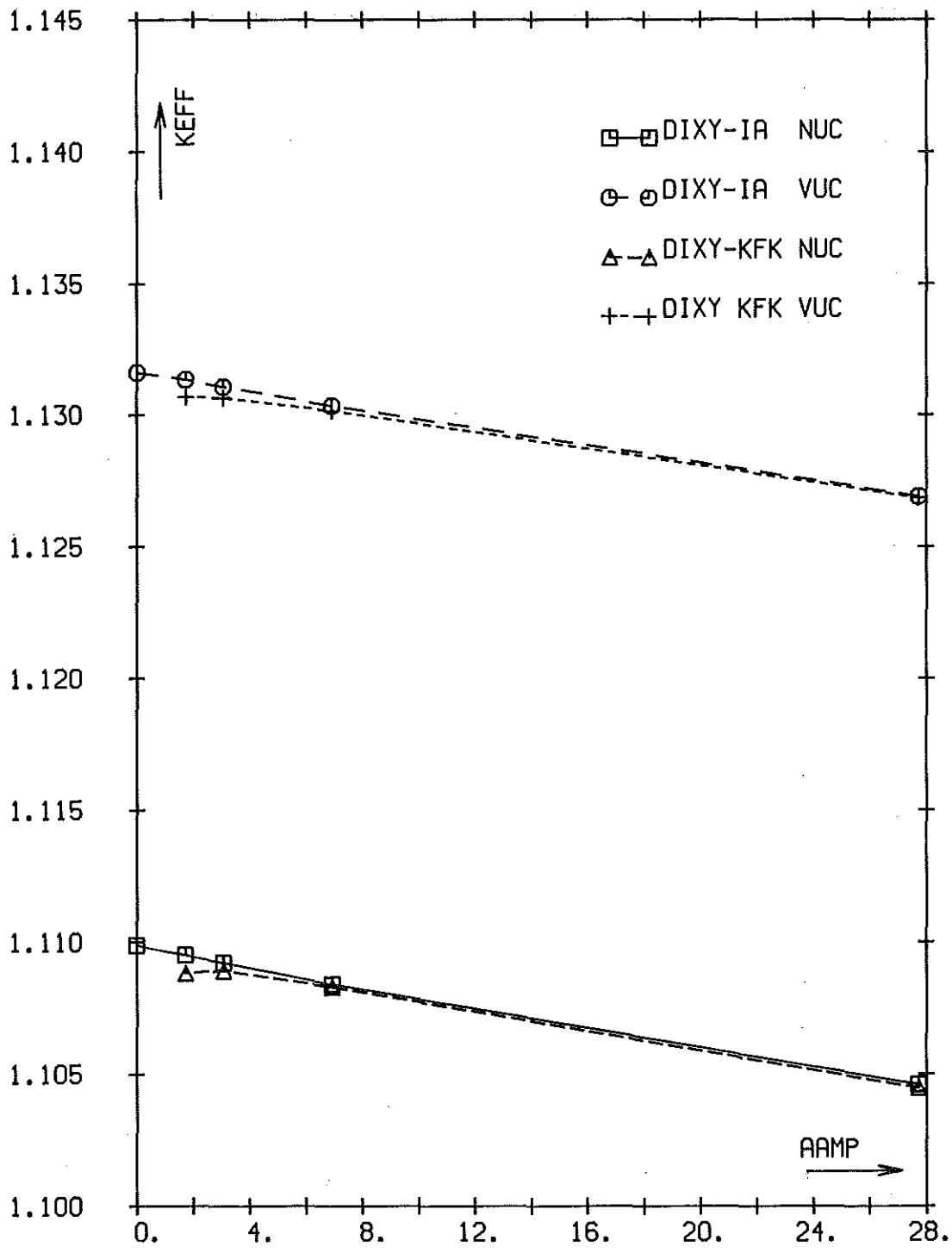

FIG. 1 KEFF AS FUNCTION OF AAMP

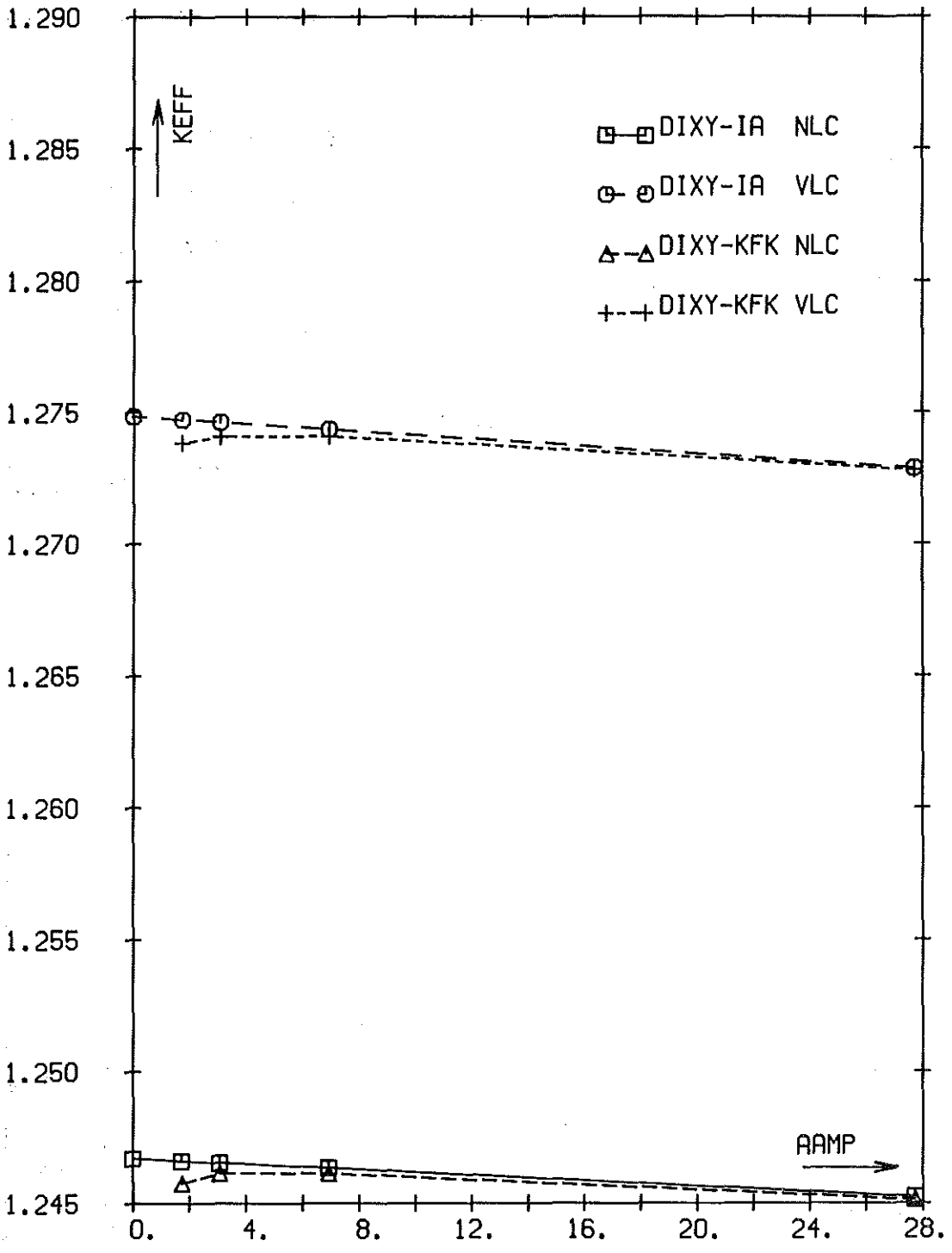

FIG. 2 KEFF AS FUNCTION OF AAMP

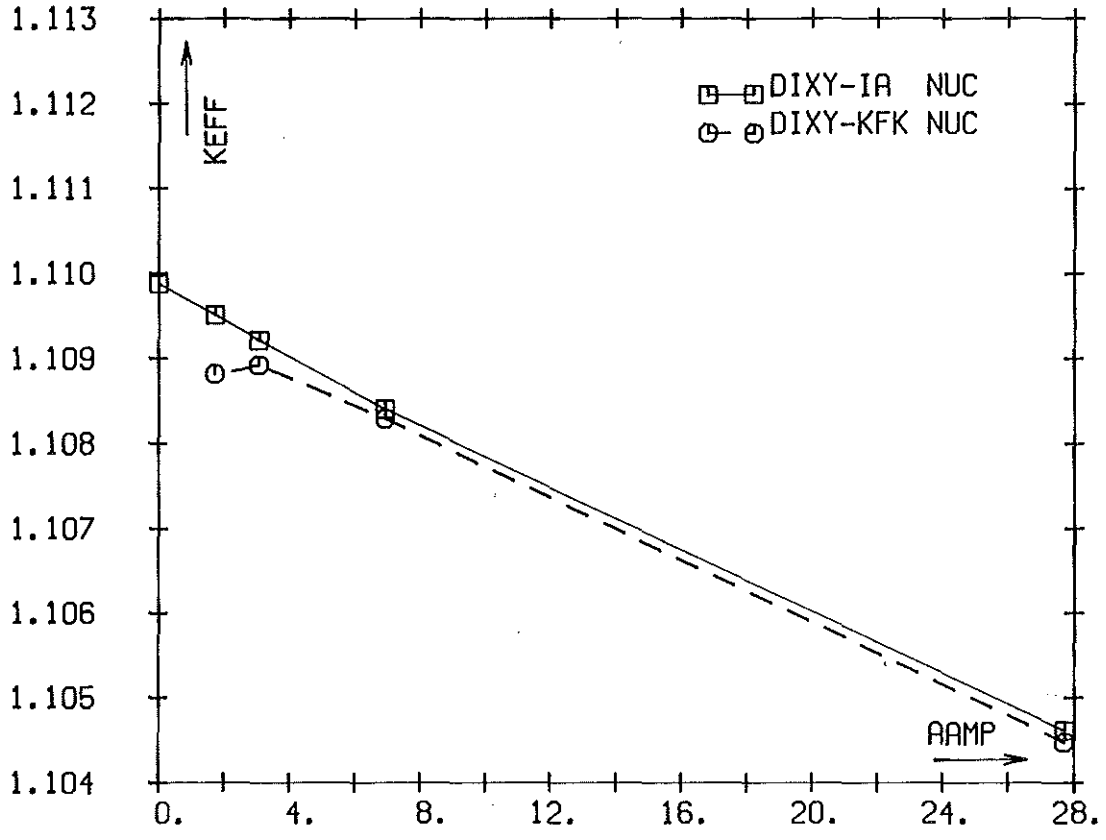

FIG. 3 KEFF FØR NUC AS FUNCTIØN ØF AAMP

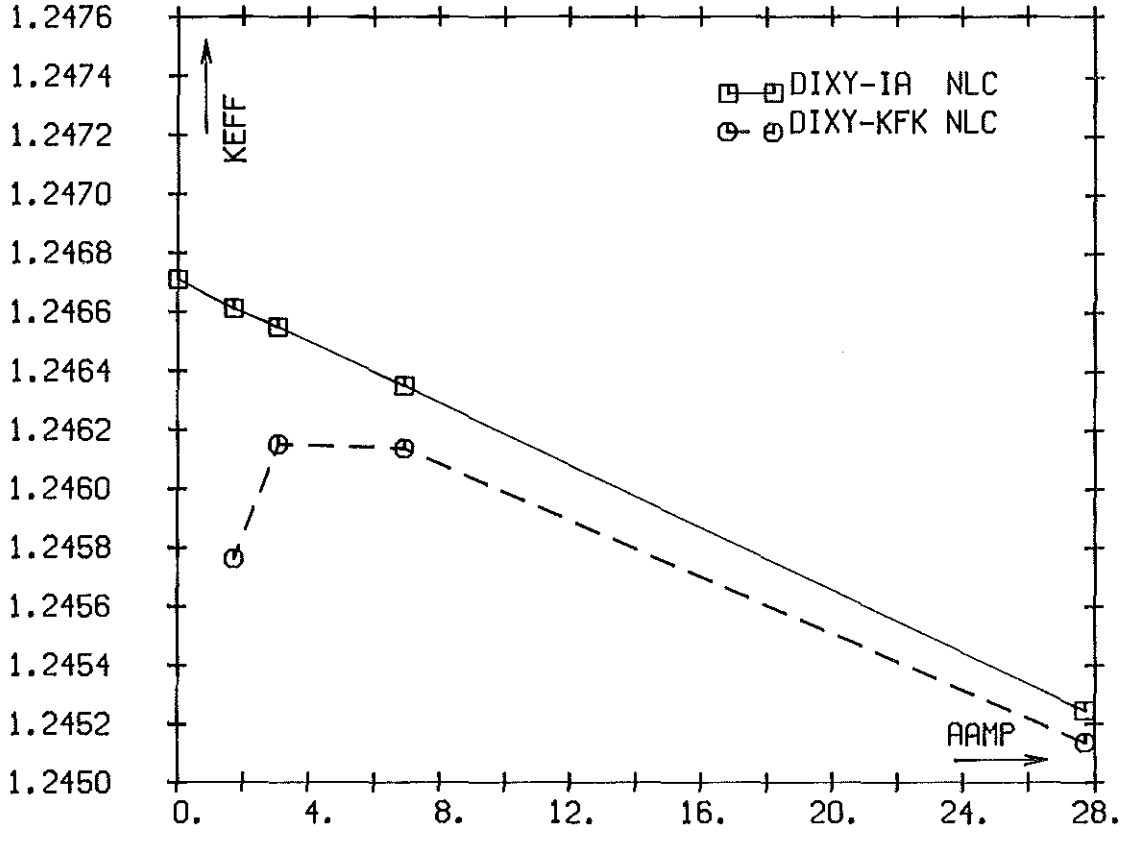

FIG. 4 KEFF FØR NLC AS FUNCTIØN ØF AAMP

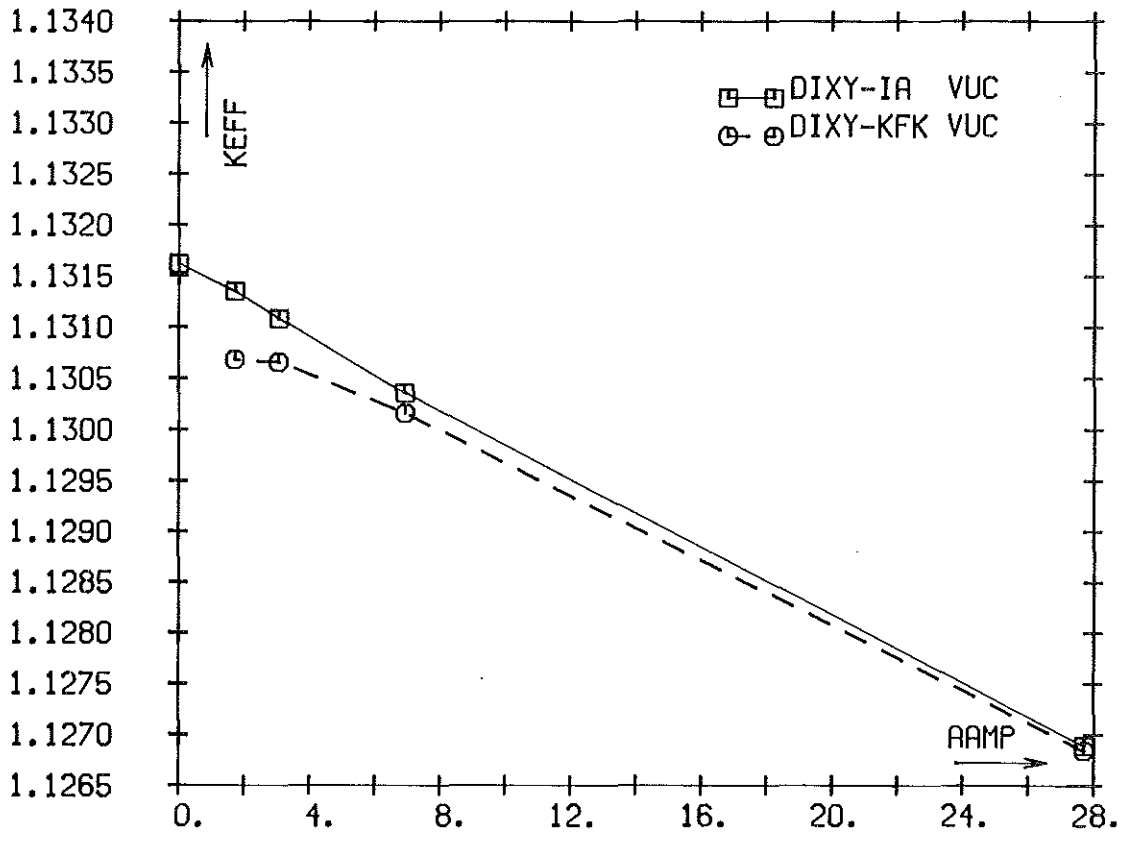

FIG. 5 KEFF FØR VUC AS FUNCTIØN ØF AAMP

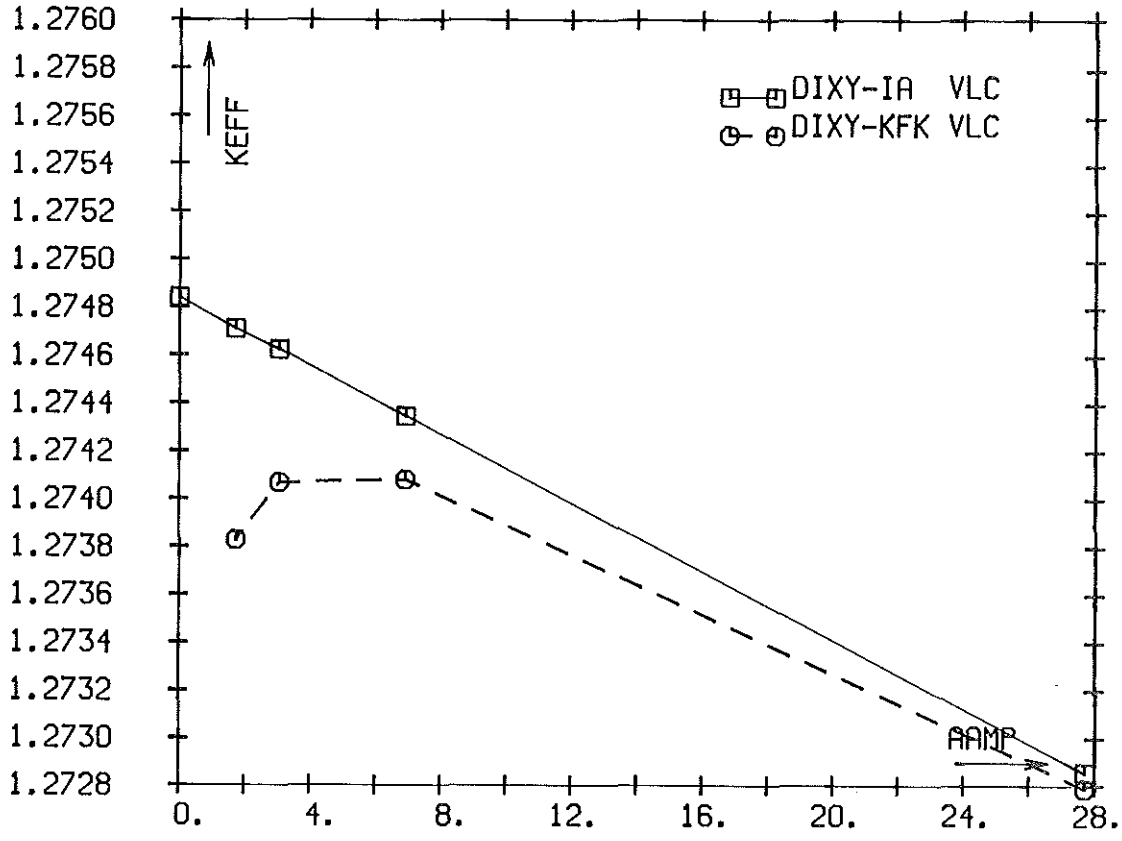

FIG. 6 KEFF FØR VLC AS FUNCTIØN ØF AAMP

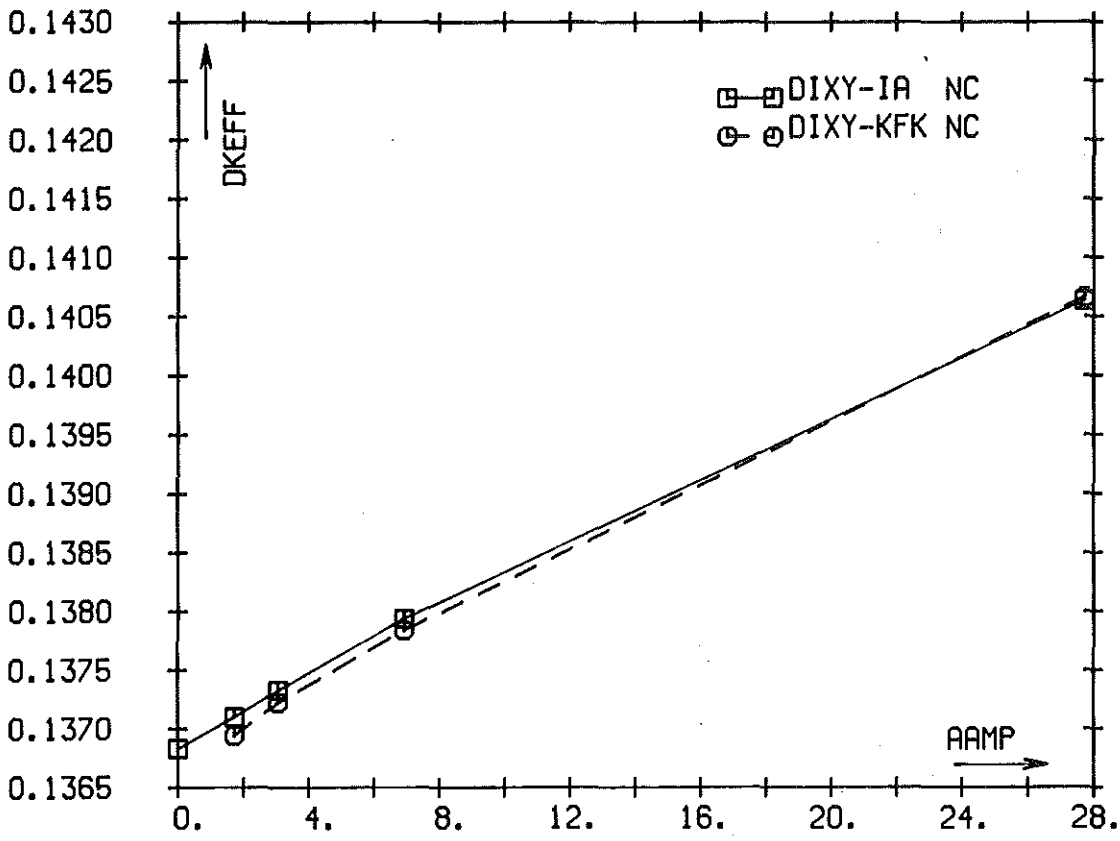

FIG. 7 CONTROL ROD WORTH FOR NORMAL CORE

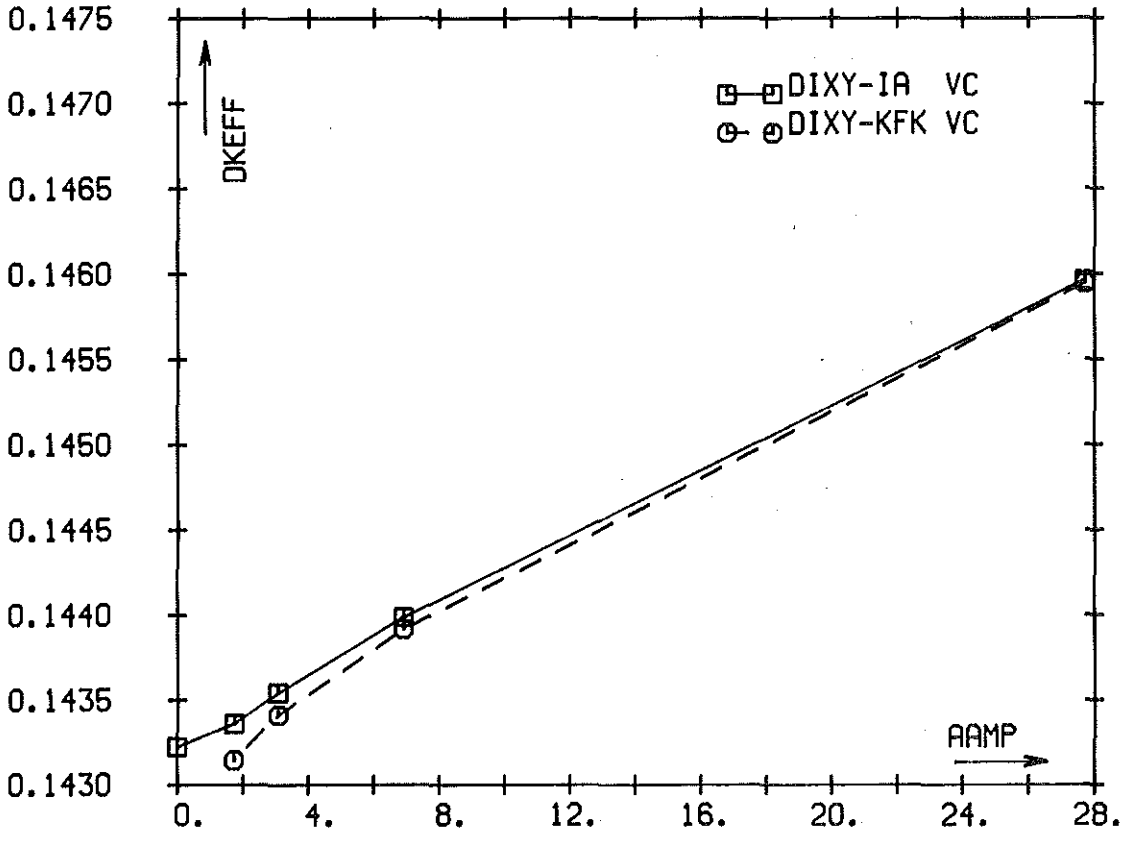

FIG. 8 CONTROL ROD WORTH FOR VOIDED CORE

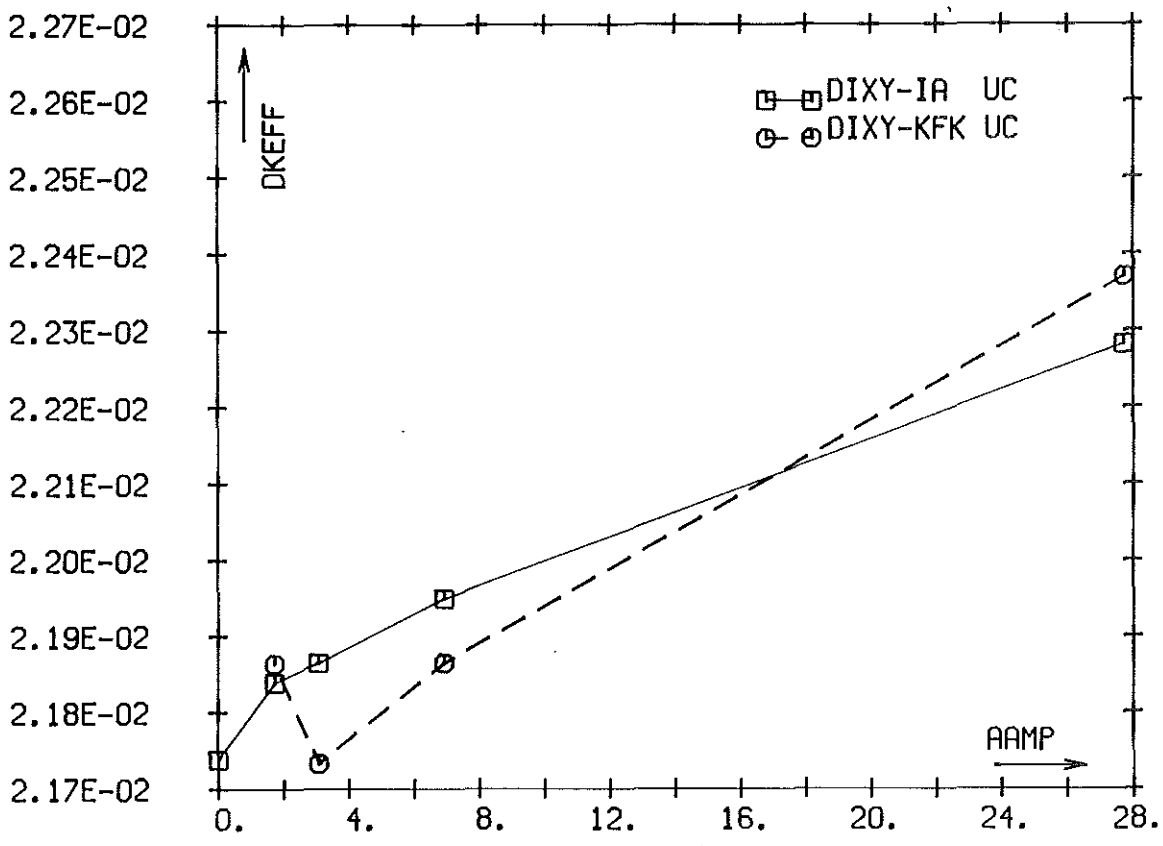

FIG. 9 NA-VØID REACTIVITY FØR UPPER CØRE

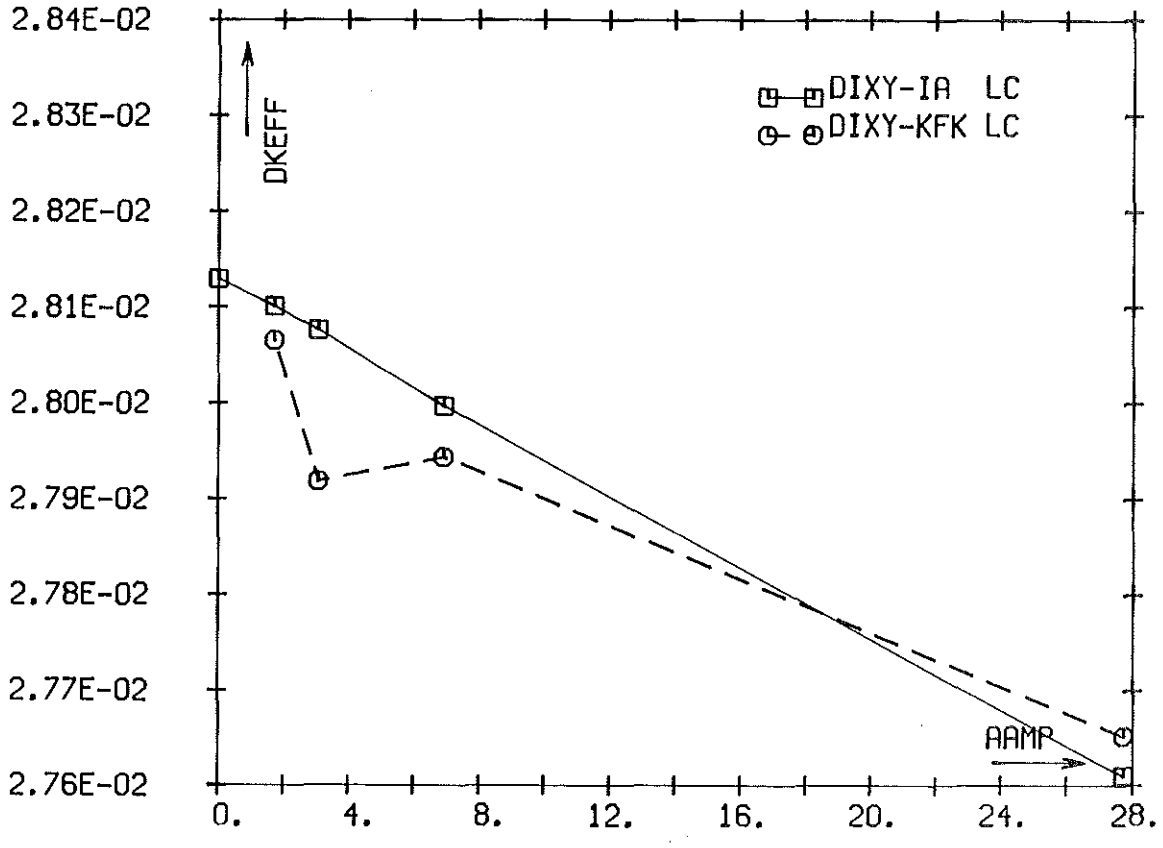

FIG. 10 NA-VØID REACTIVITY FØR LØWER CØRE

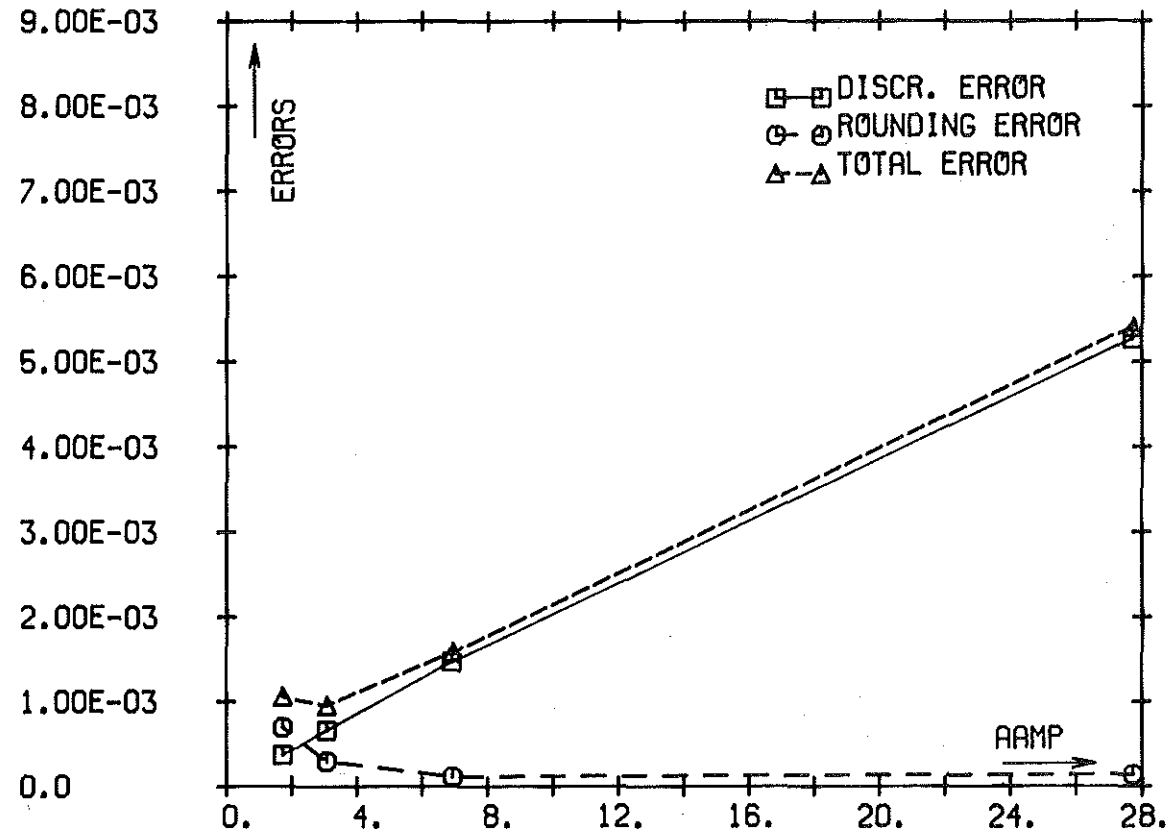

FIG. 11 DISCR. ROUNDING AND TOTAL ERROR (NUC)

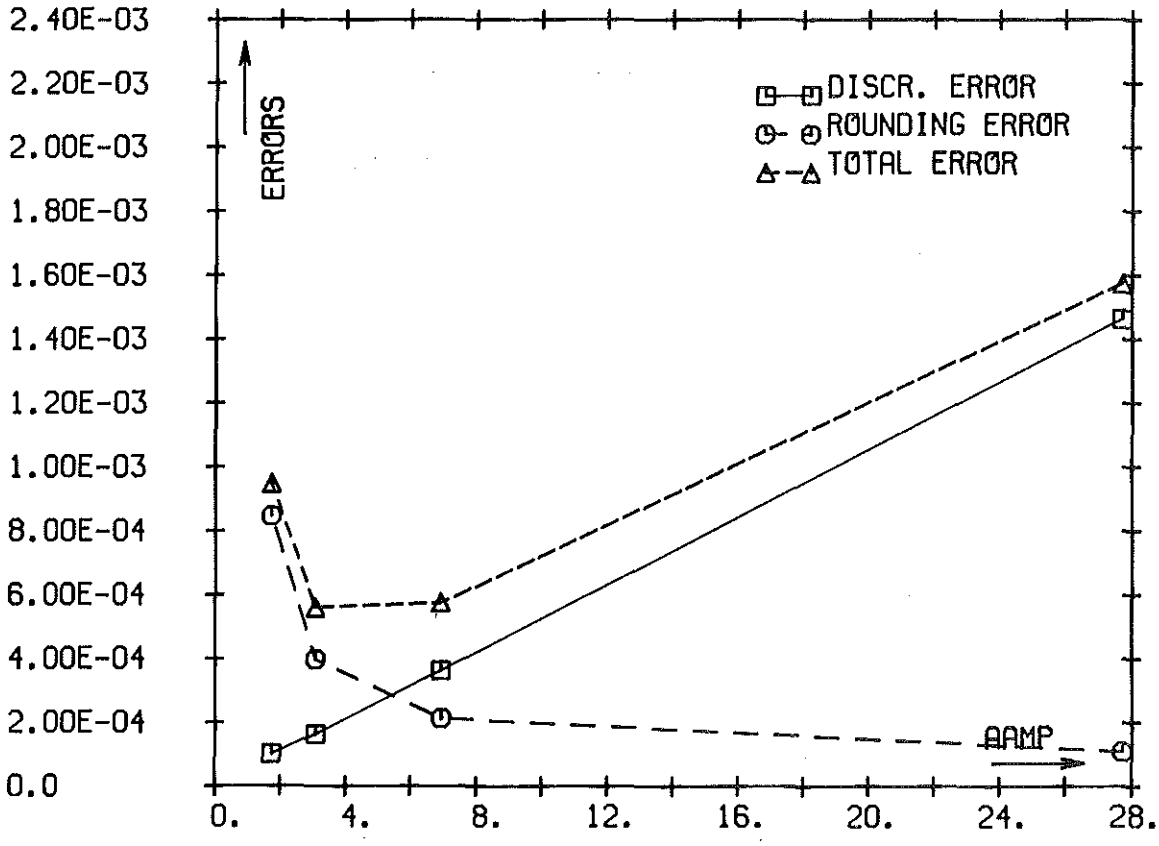

FIG. 12 DISCR. ROUNDING AND TOTAL ERROR (NLC)

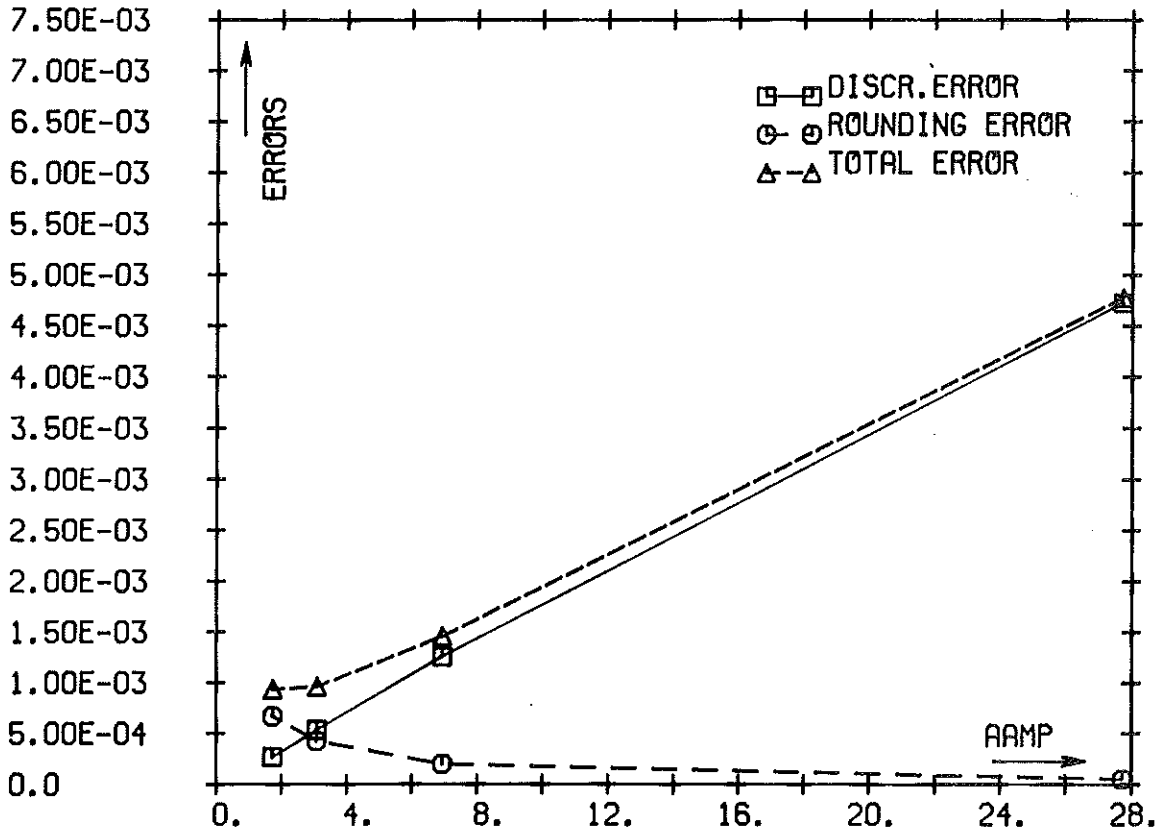

FIG. 13 DISCR. ROUNDING AND TOTAL ERROR (VUC)

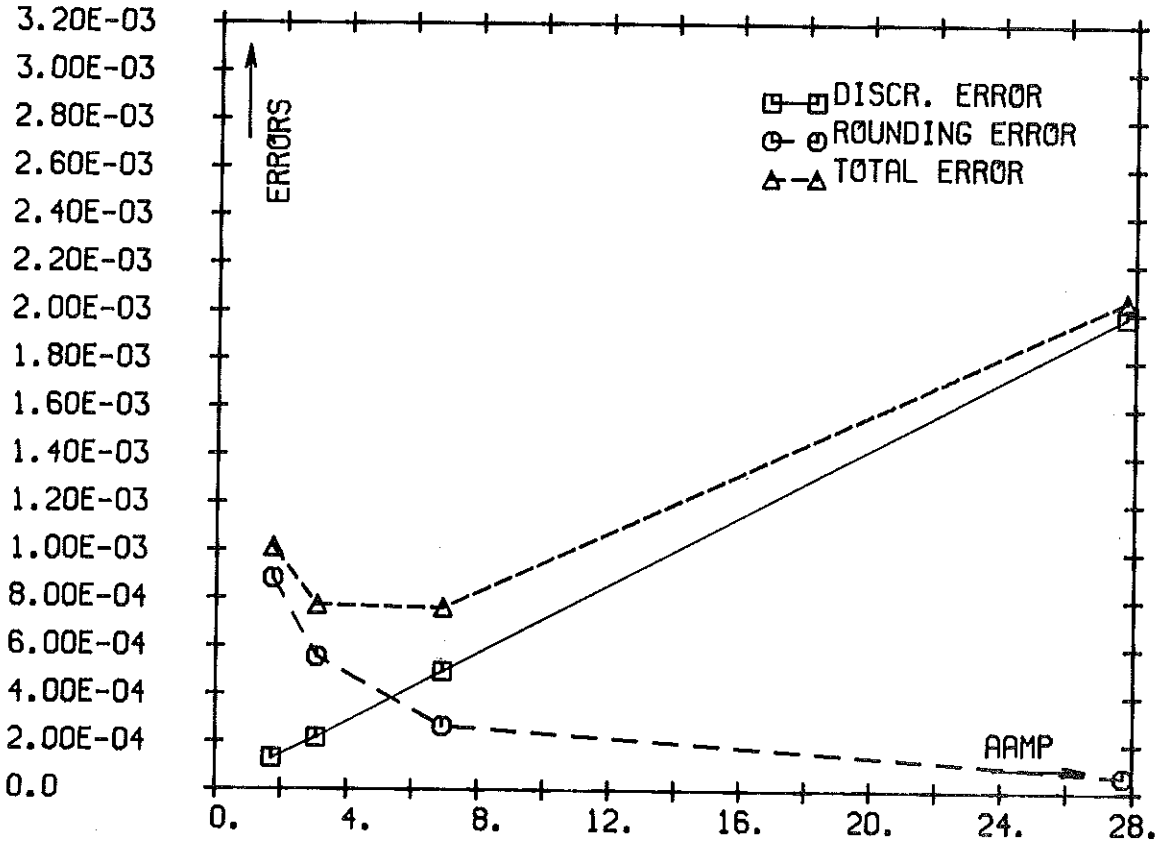

FIG. 14 DISCR. ROUNDING AND TOTAL ERROR (VLC)

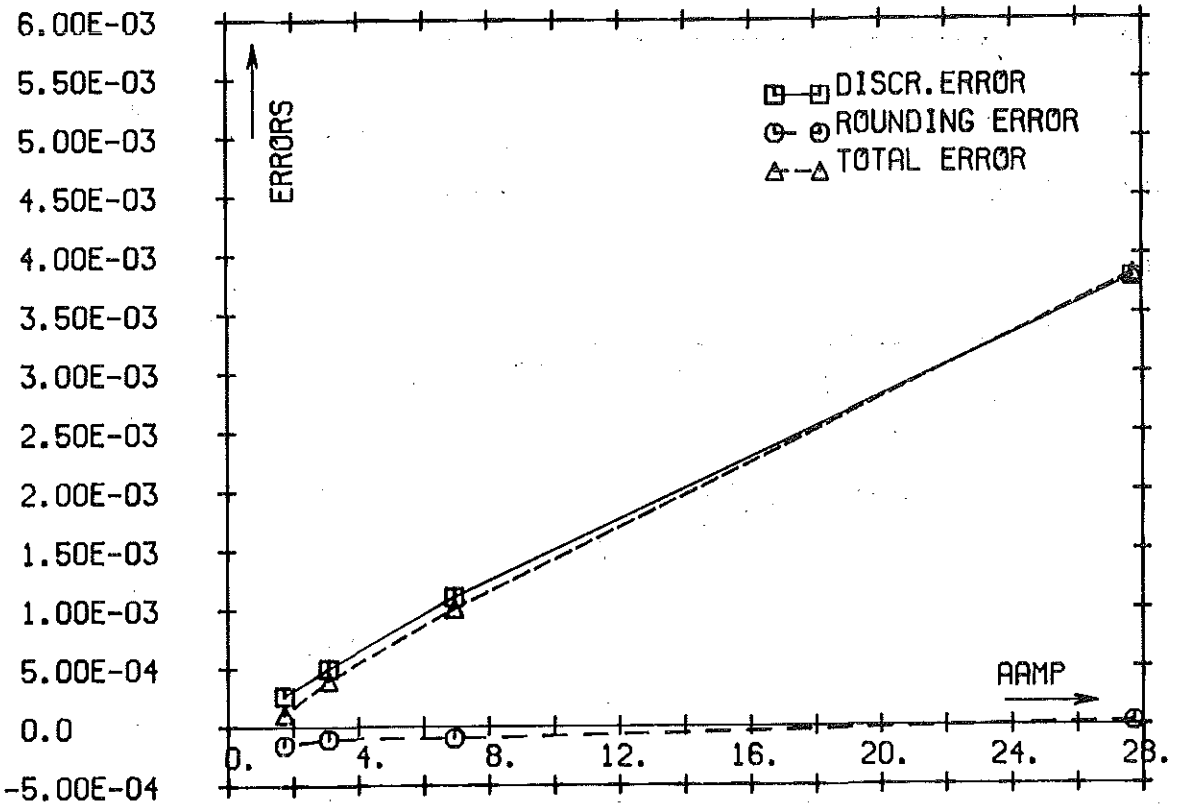

FIG. 15 ERRORS FOR CONTROL ROD WORTHS (NORMAL CORE)

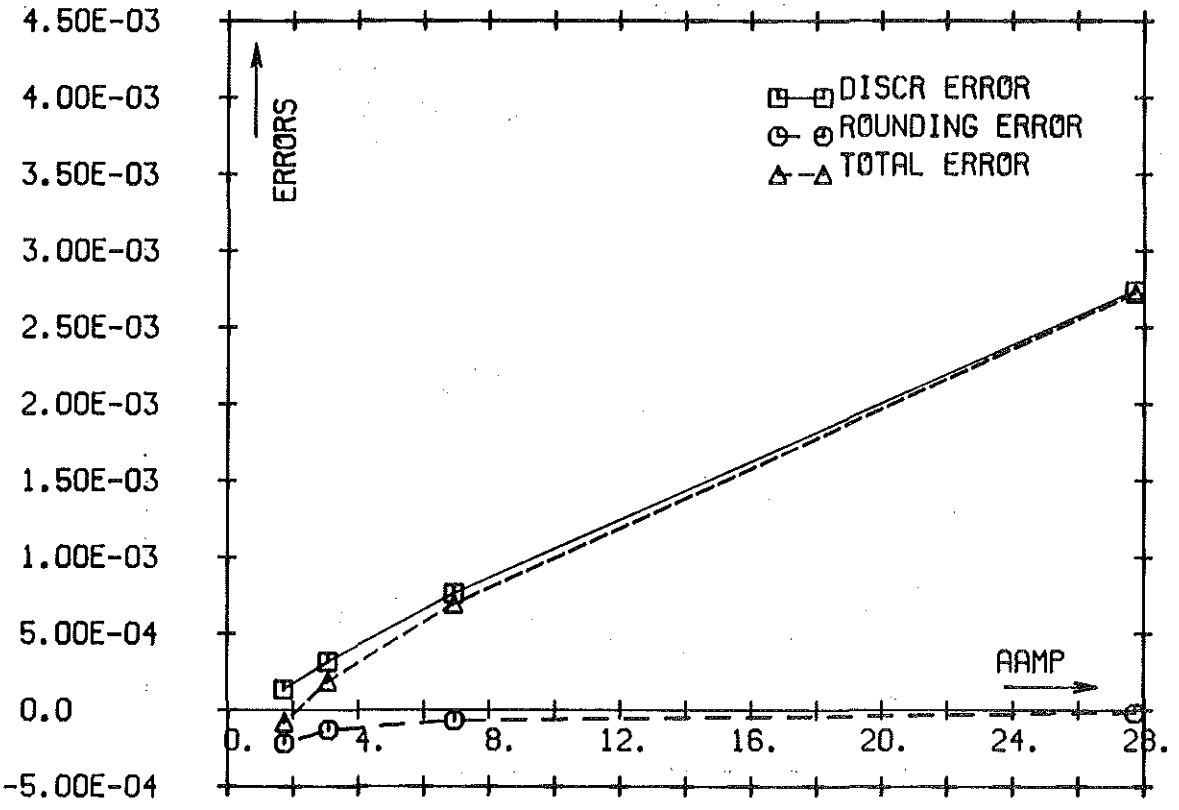

FIG. 16 ERRORS FOR CONTROL ROD WORTHS (VOIDED CORE)

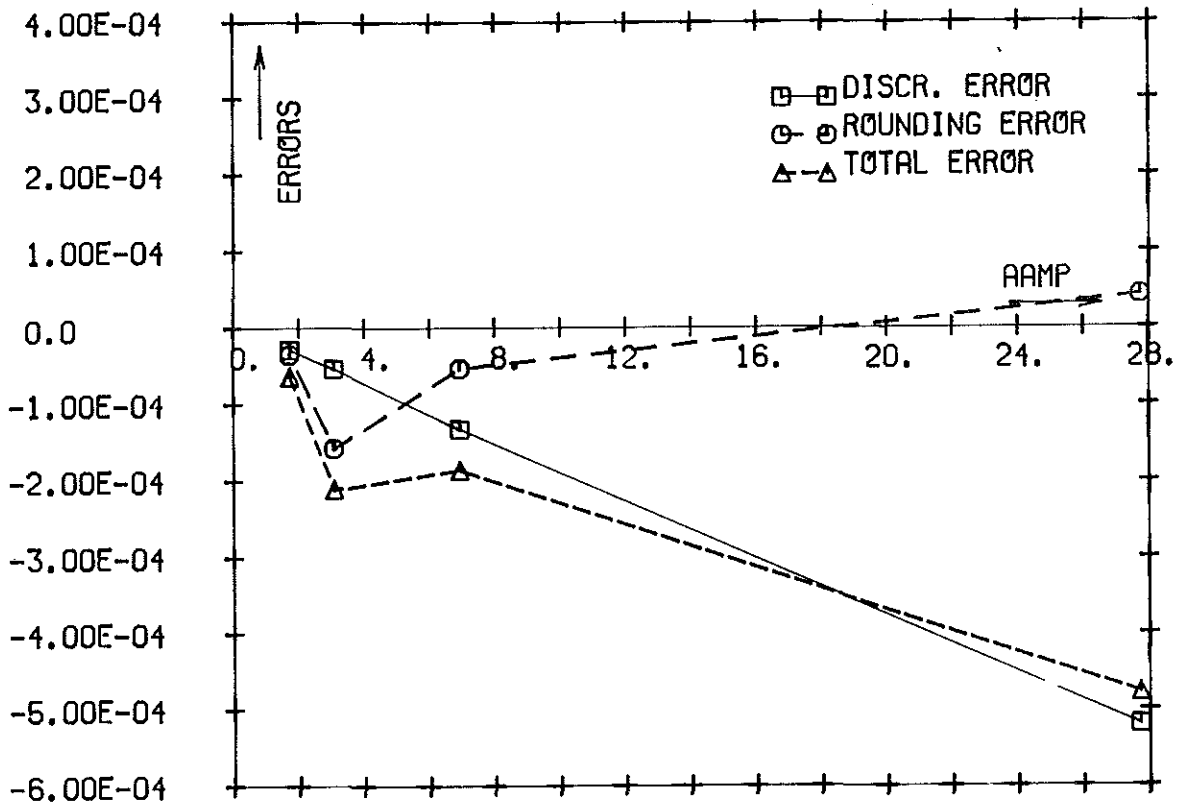

FIG. 17 ERRORS FOR NA-VOID REACTIVITY (LOWER CORE)

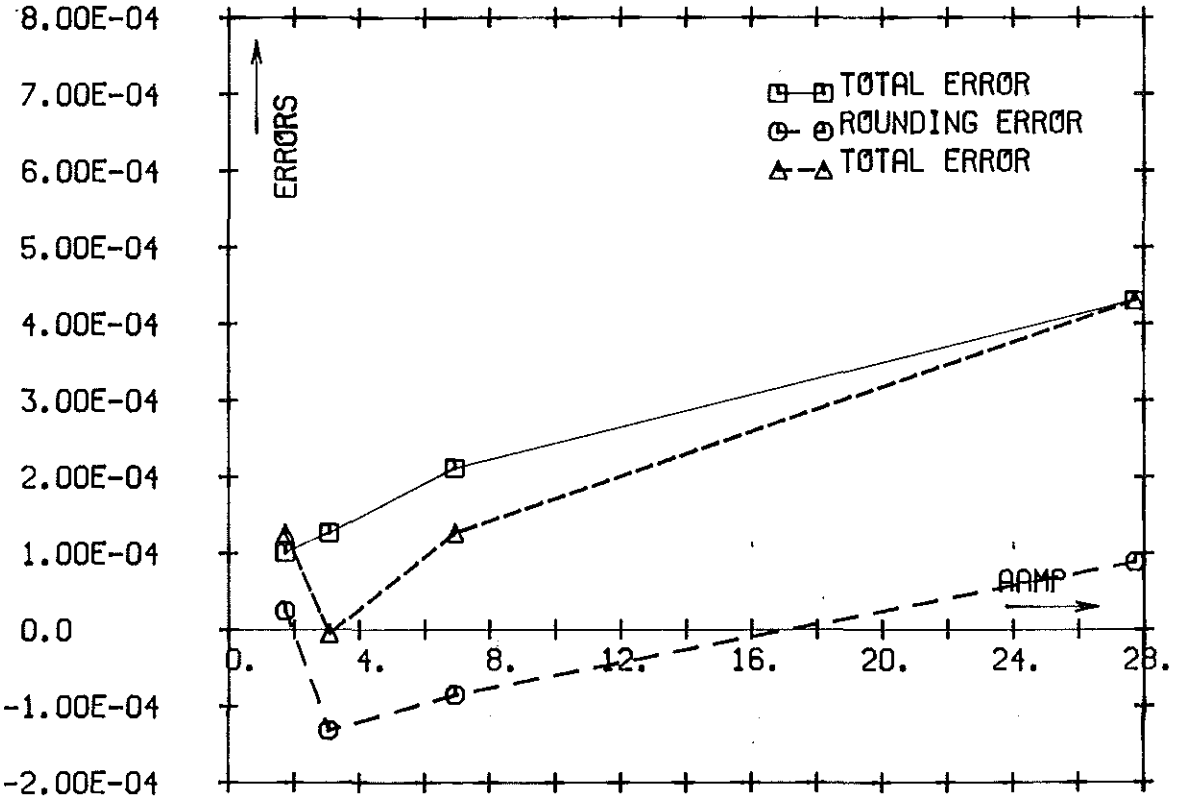

FIG. 18 ERRORS FOR NA-VOID REACTIVITY (UPPER CORE)

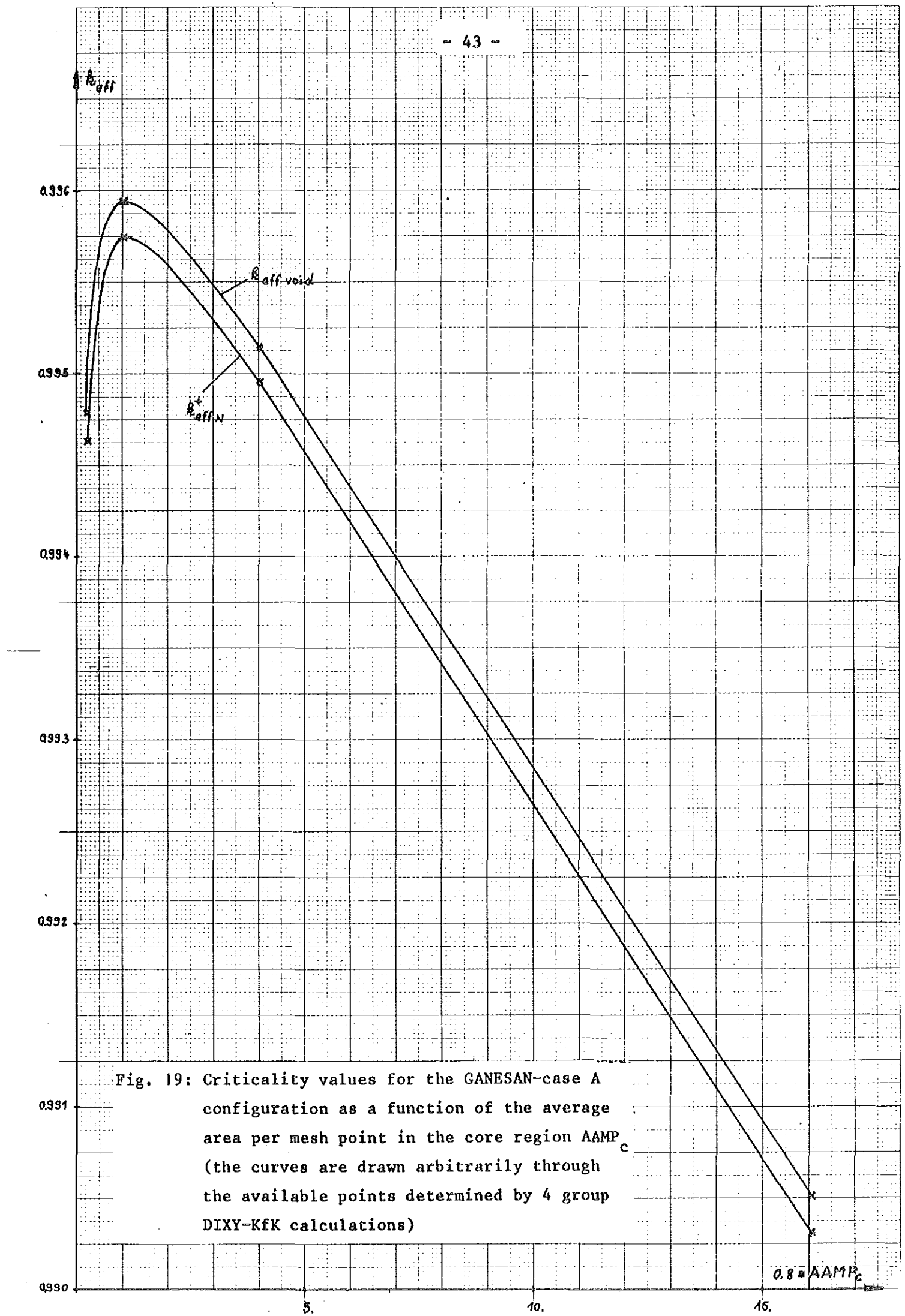

Fig. 19: Criticality values for the GANESAN-case A configuration as a function of the average area per mesh point in the core region AAMP$_c$ (the curves are drawn arbitrarily through the available points determined by 4 group DIXY-KfK calculations)