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Institut für Neutronenphysik und Reaktortechnik Projekt Schneller Brüter

The KFKINR-Set of Group Constants; Nuclear Data Basis and First Results of its Application to the Recalculation of Fast Zero-Power Reactors

compiled by E. Kiefhaber



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GESELLSCHAFT FÜR KERNFORSCHUNG M.B.H. KARLSRUHE

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#### KERNFORSCHUNGSZENTRUM KARLSRUHE

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The KFKINR-Set of Group Constants; Nuclear Data Basis and First Results of its Application to the Recalculation of Fast Zero-

Power Reactors

compiled by E. Kiefhaber

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#### Abstract

The preparation of the MOXTOT-set in 1969 was a first step in the desired direction of improving the group constants used for nuclear calculations of fast reactors. Using this data-set, it was possible to predict the criticality of all zero-power reactor-assemblies studied as test cases at that time within an uncertainty limit of  $\pm 2 \%$ . Further improvements superceding the MOXTOT-set have been necessary in order to reduce the uncertainty range for the criticality prediction and to improve the prediction of other important quantities besides criticality, e.g. reaction rates which are important for the breeding properties of fast power reactors. For the test of the improved set of group constants, named KFKINR-set, we have primarily used the same critical assemblies which were taken for the test of the preceding MOXTOT-set. The important changes in the group constants with respect to the MOXTOT-set, which was used as starting point, concern mainly the heavy isotopes which are important for fast breeder reactors, especially Pu239, U238, U235, and Pu240. For the determination of the group constants for the elastic down-scattering we have used as the weighting spectrum the collision density of a typical sodium cooled fast reactor, namely that of the SNR.

The complete nuclear data basis of the improved group constants is described in chapter II. First results for the recalculation of fast critical assemblies are presented in chapter III. Some essential characteristics of the new set of group constants and the results obtained by its first test applications are summarized in chapter IV. In the Appendix some remarks on the methods of calculation are added.

#### Zusammenfassung

Die Erstellung des MOXTOT-Satzes war ein erster Teilerfolg bei der angestrebten Verbesserung der Gruppenkonstanten, die für die nukleare Berechnung schneller Reaktoren verwendet werden. Dieser Gruppenkonstanten-Satz ermöglichte es, die Kritikalität aller seinerzeit damit untersuchten Nullenergie-Reaktoranordnungen auf ± 2 % genau vorherzusagen. Weitere, über den MOXTOT-Satz hinausgehende Verbesserungen waren jedoch notwendig, um den Unsicherheitsbereich für die Kritikalitätsvorhersage zu verkleinern. Daneben sollte auch die Vorhersage anderer Größen wie z.B. von Reaktionsraten verbessert werden, um die Bruteigenschaften genauer bestimmen zu können. Für den Test des verbesserten Satzes von Gruppenkonstanten, der KFKINR-Satz genannt wurde, haben wir zunächst die gleichen kritischen Anordnungen benutzt, die bereits bei den zum MOXTOT-Satz führenden Studien verwendet wurden, der die Grundlage für den verbesserten Datensatz bildete. Die hauptsächlichen Änderungen der Gruppenkonstanten betrafen die schweren Isotope, die für schnelle Brutreaktoren wichtig sind, insbesondere Pu239, U238, U235 und Pu240. Als Wichtungsspektrum zur Bestimmung der Gruppenkonstanten für die elastische Abwärtsstreuung haben wir die Stoßdichte eines typischen natriumgekühlten schnellen Reaktors, nämlich des SNR's, benutzt.

Die Beschreibung der nuklearen Datenbasis des KFKINR-Satzes ist in Kapitel II enthalten. Erste Ergebnisse von Testrechnungen für Reaktoranordnungen sind in Kapitel III angegeben. Wesentliche Merkmale des neuen Gruppenkonstantensatzes und der damit erzielten Resultate sind in Kapitel IV zusammengefaßt. In Anhang finden sich einige Bemerkungen bezüglich der Berechnungsmethoden.

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#### I. INTRODUCTION

One basic requirement for the design of large fast power reactors is the sufficiently accurate and reliable prediction of the important nuclear parameters e.g. critical mass, breeding ratio, Doppler-coefficient, coolant void coefficient etc. The presently existing methods of calculation and, especially, the nuclear data used are not completely satisfactory in this respect. Therefore it has been and is still necessary to check the methods and data by comparing the results of calculations with corresponding experimental results. This, eventually, gives rise to refinements of the methods and to improvements of the data, which has been a continuous effort of reactor physicists and related groups during the last years. The preparation of the MOXTOT-set of group constants in 1969 /8/ was a remarkable step in the direction of improving the nuclear data used for the calculation of fast reactors. Using this data-set, it was possible to predict the criticality of all zero-power reactor-assemblies studied as test cases at that time within an uncertainty limit of  $\pm 2$  %. Further improvements superceding the MOXTOT-set have been necessary in order to reduce the uncertainty range for the criticality prediction and to improve the prediction of other important quantities besides criticality, e.g. reaction rates which are important for the breeding properties of fast power reactors. For the test of the improved set of group constants, named KFKINR-set, we have primarily used the same critical assemblies which were taken for the test of the preceding MOXTOT-set. The important changes in the group constants with respect to the MOXTOT-set, which was used as starting point, concern mainly the heavy isotopes which are important for fast breeder reactors, especially Pu239, U238, U235, and Pu240. For the determination of the group constants for the elastic down-scattering we have used as the weighting spectrum the collision density of a typical sodium cooled fast reactor, namely that of the SNR. It has been shown that it is important to take into account the precise form of the energy dependence of the fission neutron spectrum of different isotopes.

In this report we have tried to document in some detail the nuclear data basis of the improved group constants. First results of test-recalculations for experimental results obtained in fast zero-power reactors are also presented so that one can see the improvements obtained and the range of uncertainty still present for the prediction of important nuclear reactor

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parameters. Some remarks on the methods of calculation are added in the Appendix.

#### II. NUCLEAR DATA BASIS OF THE GROUP CONSTANTS

#### II.1 U238

a) σ<sub>tot</sub>

Our new group constants for  $\sigma_{tot}$  of U238 were based on the following new measurements and evaluations: in the energy range from 0.2 - 4 MeV (groups 3, 4, 5, 6, 7) on the measurements of CABÉ et.al. /1/ and on the results presented by LAMBROPOULOS /2/ which are both generally in agreement with the recent evaluation of PITTERLE /3/ in this range. In the range between 0.4 - 1.4 MeV these new values are confirmed by the recent experimental results of KOPSCH /4/ and in the range from 0.2 - 0.8 MeV they are in agreement with the rather old data of MEADS /5/ (see also e.g. /6/ Fig. U8-C2) and with data from WHALEN given in /3/ Fig. 6.

Recent Auerbach-Moore optical model calculations by YIFTAH /7/ also indicated an increase in the total cross section of U238 from 50 keV to 1 MeV which corresponds favourably well to the data just mentioned before.

Due to the changes indicated before, our group constants for  $\sigma_{tot}$  (U238) were increased in the energy range from 0.2 MeV to 1,4 MeV and slightly reduced from 1.4 to 4 MeV compared to the previously used values.

b) o<sub>capt</sub>

In /8/ our capture cross section of U238 below 100 keV was based on the MOXON-data /9/. Due to the history of the generation of the set of group constants discussed in /8/ there were still included very low values for the capture cross section of U238 in the energy range from 100 - 800 keV which were based essentially on the low fission cross section of U235

given by POENITZ. This inconsistency has now been removed and an additional small correction has been applied.

From 100 - 800 keV we derived mean values for the ratio  $\sigma_{\gamma}(U238)/\sigma_{f}(U235)$  from the various series of measurements shown in the publications of POENITZ /10, 11/ and with our values of  $\sigma_{f}(U235)$  which are essentially based on WHITE's data we determined consistent values for  $\sigma_{c}(U238)$  in the energy range mentioned taking also into account the results of FRICKE et.al. /12/ and the evaluation of BYER and KON'SHIN /13/ in the extended energy range from 0.05 - 10 MeV. In the energy range from 1 - 2.15 keV (group 14) and from 21,5 - 100 keV (group 9 and 10) we have taken into account the experimental result of SILVER et.al. presented at the ANS summer meeting in 1970 which is in good agreement with SOWERBY /14/ in the energy range 21,5 - 100 keV and is somewhat higher than MOXON's data.

It seems important to mention, that the resonance parameters and therefore also the resonance self-shielding factors have not been changed for the new set of group constants. This has to be postponed to a KEDAKreevaluation of the corresponding data.

#### Comparison with ENDF/B-data

Between 1 - 100 keV our capture group constants for U238 which are based on the MOXON-data are rather low compared to the new ENDF/B evaluation by PITTERLE /3/. Above 100 keV our data are in better agreement with the ENDF/B data.

#### Comparison with other data

Between 0.1 - 1 MeV we find reasonable agreement with the results of SOWERBY /14/ and of POENITZ /11/ which becomes even better in the energy range from 10 - 100 keV. Between 1 - 10 keV our (MOXON)-data agree rather well with the experimental results presented by SILVER.

But there is a marked discrepancy to the recent experimental results obtained at GGA by FRICKE et.al. /15/. At present this systematic discrepancy between different experimental results is unexplained.

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In order to get rid of this discrepancy DAVEY increased the MOXON-data by 15 % in his evaluation /16/. Further careful precision measurements seem to be necessary to clarify and remove this discrepancy.

## c) σ fiss

Compared to the data given in /8/ we have made only one additional change: in the energy range from 2.5 to 4 MeV it was felt necessary to reduce our value somewhat because in /8/ the renormalization of the Los Alamos data has been done for U235 and Pu239 between 2.5 and 10.5 MeV but for U238 only between 4.0 and 10.5 MeV. With the inclusion of this new value our group constants for  $\sigma_{\rm f}$ (U238) are in good agreement with the evaluation of BRESESTI /17/ and with the new ENDF/B-evaluation by PITTERLE /3/ in the whole energy range of interest for fast reactors.

### d) $\sigma_{\text{inel}}$ , $P_{\text{inel}}$ (E $\rightarrow$ E')

In the past there have been several indications (see e.g. /18, 19/) from the evaluation of integral data that the cross section for inelastic scattering of U238 has to be reduced. We have now used below 1.2 MeV the rather old experimental results of SMITH /20/ which are generally in acceptable agreement with the Russian ABN-data. At the Helsinki-Conference in 1970 POENITZ /11/ reported a value of 2.87 barns at 1.6 MeV deduced from measurements of SMITH which is about 13 % lower than the corresponding result of BARNARD. Generally the detailed measurements of BARNARD /21/ which were confirmed by his recent measurements /22/ are higher in the region of the first few excited levels than the data of SMITH /20/. The evaluation of SCHMIDT /6/ and probably also the recent ENDF/B evaluation of PITTERLE /3/ rely heavily on the data of BARNARD below 1.2 MeV. It would be very helpful to have an independent careful measurement of the cross section for inelastic scattering of U238 and the corresponding energy transfer below about 1.2 MeV to see if BARNARD's results can be reproduced.

Above 1.4 MeV our previous data /8/ have been reduced in the average by about 20 % in accordance with the studies of KALLFELZ /18/. In addition to the changes in  $\sigma_{inel}$  we also changed the energy distribution of the

inelastically scattered neutrons. For the statistical inelastic scattering we used the Maxwellian distribution with a temperature  $\Theta(E) = 0.206 \ E^{1/2}$  taken from the evaluation of PITTERLE /3/ which is based on a fit to the measurements of BATCHELOR /23/. This means that in our formula for  $\Theta(E) = (E/\gamma A)^{1/2}$ ,  $\gamma$  has now to be changed from 0.16 MeV<sup>-1</sup> to 0.099 MeV<sup>-1</sup>.

Below 1.4 MeV we used the inelastic scattering probabilities taken from the Russian ABN group-set to replace our previously used data. Further precise measurements in the region of the first few excited levels will show whether this replacement is justified or not.

#### e) other group constants

The other group constants not mentioned here explicitly have been kept constant except for  $\sigma_e$  which has been changed in such a way that the new value for  $\sigma_{tot}$  is the sum of all partial cross sections.

#### II.2 U235

### a) $\sigma_{tot}$

The new group constants for  $\sigma_{tot}$  of U235 were based on the measurements of CABÉ et.al. /1/ in the energy range from 0.2 - 6.5 MeV (group 2, 3, 4, 5, 6, 7). In the whole energy range the new values show a slight increase compared to the previously used values.

Below 1 keV the group constants for  $\sigma_c$  (U235) have been reduced as mentioned in the next paragraph. In this energy range the group constants for elastic scattering have not been changed but  $\sigma_{tot}$  has been reduced according to the reduction in  $\sigma_c$ .

b) σ<sub>capt</sub>

Above 1 keV our values for  $\alpha(=\sigma_c/\sigma_f)$  of U235 are generally compatible with the recent measurements of /24/, /25/, /26/. Therefore above 1 keV  $\alpha$  has not been changed with the exception of the energy range from 20 - 50 keV where the preliminary results of BANDL and FRÖHNER /26/ indicate somewhat lower  $\alpha$ -values in agreement with the results given

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by KUROV /24/.

One should, however, mention that the group constants for  $\sigma_c$  (U235) have been changed in accordance with changes in the values for  $\sigma_r$ (U235).

Below 1 keV our values for  $\alpha(U235)$  have definitely to be modified as already indicated in /27/. From the results of de SAUSSURE /28/ rough estimates of  $\alpha(U235)$  below 300 eV have been deduced. These data have then been used together with the unchanged data for  $\sigma_{f}(U235)$  to determine improved group constants for  $\sigma_{c}(U235)$  below 200 eV.

### c) o<sub>fiss</sub>

In the energy range between 1.4 - 2.5 MeV (group 4) and between o.4 - o.8 MeV (group 6) the group constants for  $\sigma_f(U235)$  have been slightly reduced, so that the new values show an improved agreement with the data of WHITE /29/. The reduction is so small, that both, the old and new group constants are within the experimental range of uncertainty of the KEDAK - as well as the WHITE-data.

The recent  $\sigma_{f}$ -measurement of KÄPPELER /30/ who reported at 440 and at 530 keV a value of 1.17 ± 3.5 % is also in good agreement with our improved group constant for  $\sigma_{f}(U235)$  in this energy range. Recent publications of SOWERBY /14/, SZABO /31/, POENITZ /11/ and BLONS /32/ seem to indicate that our previous values for  $\sigma_{f}(U235)$  below 400 keV have to be decreased. This has been done in the energy range from 1 - 400 keV with special weight given to the measurements of BLONS. From the corresponding figures in the reports of POENITZ /11/ and of DAVEY /33/ and from the measurements of SZABO /31/ it can be seen that in the energy range between 20 - 100 keV even lower group constants for  $\sigma_{f}(U235)$  than our presently accepted values seem to be possible.

The details in the structure of both the fission cross section of U235 and the  $\alpha$ -values as indicated e.g. in the measurements of de SAUSSURE /28/ PATRICK (see /14/), BLONS /32/ and BOWMAN (see /11/) could not be considered here when new group constants have been determined. This must be postponed to a future careful evaluation of this phenomena for the KEDAK-file.

#### d) v

At the Helsinki-Conference in 1970 some new results on the energy dependence of v(E), the mean number of secondary neutron per fission, have been reported: the measurements of SOLEILHAC et.al. /34/ and the compilations or evaluations found in the papers of DAVEY /33/ and POENITZ /11/. Besides this a new evaluation is underway at Karlsruhe /35/ for the whole energy range from thermal to 14 MeV which takes also into account the reevaluation of the thermal value done by HANNA, WESTCOTT et.al. /36/ and the renormalization of the  $\bar{\nu}$ -value for Cf252. Our improved values of the group constants for  $\bar{\nu}(U235)$ have been determined essentially by using preliminary results of the present Karlsruhe evaluation /35/. In the energy range from 0.2 -1.4 MeV our improved values are in good agreement with the results of SOLEILHAC /34/. From the reports of DAVEY /33/ and POENITZ /11/ somewhat larger values for  $\bar{\nu}(U235)$  would have been deduced in the energy range from 0.1 - 0.4 MeV than those presently recommended by us.

e)  $\sigma_{and}$  and other group constants

Below 1 keV the group constant for elastic scattering has been kept constant, as already mentioned in the paragraph reporting on  $\sigma_{tot}$ . Above 1 keV the elastic scattering group constant has been adjusted in such a way that the new value for  $\sigma_{tot}$  is the sum of all partial cross sections.

All other group constants not mentioned here explicitly have not been changed.

#### II.3 Pu239

#### General remark

Since the production of the MOXTOT-set a new evaluation of a few types of nuclear reactions for Pu239 has been performed at Karlsruhe by Miss

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HINKELMANN /37/. This evaluation has been taken as the basis for the generation of new group constants. In the following we will only describe those changes which lead to group constants differing from those generated from the recent evaluation /37/.

a) o<sub>tot</sub>

As for the other isotopes we have taken into account the recent measurements of CABÉ et.al. /1/ which are generally in good agreement with the older measurements of MEADS (see e.g. /6/ Fig. Pu9-C2). In most parts of the energy range considered (o.2 - 6.5 MeV) this leads to an increase of the group constants for  $\sigma_{tot}$  (Pu239).

# b) o capt

In the evaluation by HINKELMANN /37/ essentially the  $\alpha$ -values of GWIN have been used as the basis for  $\sigma_c$  (Pu239) in the low keV region. Since that time new and improved data have become available mainly at the Helsinki-Conference in 1970. In the high keV range (above o.4 MeV) we have now adopted the reevaluated ENDF/B-data presented by BEST et.al. /38/ taking rough estimates for  $\sigma_c$  (Pu239) from this reevaluation. In the energy range from 10 - 50 keV we have increased the  $\alpha$ -value because the results of GWIN seem to be somewhat too low in this range. This can be seen if one considers to data of SCHOMBERG et.al. /39/, or the data presented in Fig. 8 of the report of POENITZ /11/. The results of KUROV /24/ and of BANDL and FRÖHNER /26/ give the same indication.

In the energy range from 1 - 5 keV we have decreased the  $\alpha$ -value because in this range the results of GWIN seem to be somewhat too high as can be seen from references /39/, /11/, /24/.

The group constants for  $\sigma_c$  have been changed in accordance with the changes in the  $\alpha$ -values and, if necessary, in accordance with changes in  $\sigma_r$ (Pu239) discussed in the next paragraph.

In the energy range below some hundred eV our KEDAK-file does not contain the best information which at present is available from the experimental results. This is mainly due to the fact that we are primarily concerned

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with fast reactors with hard neutron spectra for which this region is of minor importance. For assemblies with softer neutron spectra the importance of this region increases and it may be that the theoretical results for the  $k_{\infty}$ -experiments SNEAK-5C and ZPRIII-55 are influenced to some extent by changes in the nuclear data in the energy region below some hundred eV.

A future evaluation in this energy range should take into account the results of LOTTIN et.al. /40/, GWIN /41/, CZIRR and LINDSEY /42/, FARRELL /43/ and the evaluation of EVATT and HUTCHINS /44/. Furtheron one should remove the presently existing inconsistency on the KEDAK-file between the tabulated microscopic cross sections and the corresponding resonance parameters in the resolved resonance region. At present this inconsistency leads in some energy ranges to remarkable discrepancies in the  $\alpha$ -value and to less severe descrepancies in the value of  $\sigma_{\rm f}$  even if averaged over the group structure of the Russian ABN-set. At present we have used in the energy range from 4.65 - 465 eV (group 16 - 21) the results derived from the inclusion of the evaluation of RIBON into an improved version of the KEDAK-file established recently by Miss HINKELMANN. This has been done for the determination of the group constants  $\sigma_{\rm f}$ ,  $\sigma_{\rm c}$  and  $\sigma_{\rm el}$  from resonance parameters.

c) o<sub>fiss</sub>

Compared to the recent evaluation by HINKELMANN only minor modifications of the fission cross section have been performed for our new set of group constants. Between 0.2 - 0.4 MeV and 0.8 - 1.4 MeV we increased our group constants for  $\sigma_{\rm fiss}$  and  $\sigma_{\rm capt}$  slightly in order to come to more acceptable values for the ratio  $\sigma_{\rm f}({\rm Pu}_{239})/\sigma_{\rm f}({\rm U}_{235})$  compared to the corresponding average values of a series of different measurements as given e.g. in the work of POENITZ /10/. The measurements of SZABO et.al. /31/ also indicates that the HINKELMANN evaluation probably gives slightly too low  $\sigma_{\rm f}$ -values in the energy region from 0.2 - 1.4 MeV. The same tendency for most of the energy region between 0.1 and 1.4 MeV can be deduced from the DAVEY-evaluation which is also shown in Fig. 5 of the work of SZABO et.al. /31/.

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An opposite tendency at least for the energy range form o.4 - 1.4 MeV seems to be indicated by the measurements of SOLEILHAC /34/ for the ratio  $\sigma_r(Pu239)/\sigma_r(U235)$ .

From the work of GWIN /41/ and the results of LEHTO /47/ we determined in the energy range from 1 - 20 keV new group constants for  $\sigma_{\rm f}$  which are most times somewhat higher than those obtained from the HINKELMANNevaluation.

For the energy range below some hundred eV essentially the same comments apply to  $\sigma_{\rm f}$  as already given in the preceding paragraph for  $\sigma_{\rm c}$ . A future evaluation should take into account the results of JAMES /46/, LEHTO /47/, GWIN /41/, LAMBROPOULOS /48/, POENITZ /10/, and of the evaluation by EVATT and HUTCHINS /44/.

For the generation of group constants below some keV one should carefully study (a) the effect of the spin-dependence of the fission width of Pu239 on the resonance self-shielding factors and their variation with temperature as discussed by KIKUCHI /49/ and (b) the effect on effective cross sections caused by the intermediate resonance parameter representation used to describe the intermediate structure of the fission cross section as discussed also by KIKUCHI /50/.

#### d) $\bar{\nu}$

The group constants for  $\bar{v}(Pu239)$  determined from the HINKELMANN-evaluation have been renormalized in the whole energy region from thermal to 10 MeV according to the new value of 3.756 for  $\bar{v}_p$  (Cf) which is somewhat lower than the previously used value of 3.764. This leads to a new thermal value of 2.8859 for  $\bar{v}_t$ (Pu239) which is about 0.2 % higher than the corresponding value of 2.8799 given in the evaluation of HANNA and WESTCOTT /36/. In the energy range from 0.2 - 1.4 MeV our new values seem to be in reasonable agreement with most recent measurements of SOLEILHAC /34/.

In the energy range above 0.5 MeV our new values are in good agreement with the evaluation of MATHER et.al. /45/ for  $\bar{\nu}_{p}$  (Pu239). Below about 0.5 MeV the small deviations between our somewhat higher values and

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the MATHER-evaluation is probably caused by the small difference in the thermal values of about 0.01.

It is probably worthwhile to mention for the sake of completeness that in the HINKELMANN-evaluation no fine structure in the energy dependence of  $\bar{v}(E)$  of Pu239 has been taken into account. One probably must wait for more precise and unique experimental results.

SCHMIDT /51/ reported that a difference in the mean number of secondary neutrons per fission has been found between spin o and spin 1 resonances; the spin o resonances giving a 2.6 % higher value than the spin 1 resonances. This effect which is probably not very important has not been taken into account in the HINKELMANN-evaluation and therefore is also neglected in our presently used group constants.

e)  $\sigma_{e1}$  and other group constants

The group constants for elastic scattering has been adjusted in such a way that the value of  $\sigma_{tot}$  is the sum of all partial cross sections.

All other group constants not mentioned explicitly have not been changed.

#### II.4 Pu240

For Pu240 only minor changes have been applied to the group constants of the MOXTOT-set. In the energy region from 1 - 10 keV  $\sigma_{fiss}$  has been increased according to values given by YIFTAH /52/ which are in acceptable agreement with the results of BYERS /53/ and PITTERLE /54/. Between 1.4 -2.5 MeV we have taken into account the recent results of SAVIN /55/ which leads to an increase in the group constant for  $\sigma_r$  in group 4.

For the sake of completeness it should be mentioned that in group 24 (0.465 - 1 eV) the group constants for infinite dilution ( $\sigma_0 = \infty$ ) and the corresponding resonance-selfshielding factors (f-factors) have been modified: because of the influence of the large resonance immediately above the upper group boundary the resonance-selfshielding factors are appreciably larger than unity especially for high temperatures and large background cross sections (large  $\sigma$ -values). This fact may cause some trouble in the interpolation of f-factors for  $\sigma_{o}$ -values different from the tabulated values. Therefore we have divided for each reaction rate (capture, fission, elastic scattering) the previously used f-factors by the f-factors for T = 2100 °C and  $\sigma_{o} = 10^{6}$  barn (the highest values used in the tables) and correspondingly multiplied the previously used infinite dilute values  $\sigma^{\infty}$  by the same values, so that the product  $\sigma^{\infty} f(\sigma_{o})$  remains unchanged but the difficulties for the interpolation of f-factors could be avoided; at the same time it is no longer possible to interpret the modified values for  $\sigma^{\infty}$  and the f-factors separately in the usual manner.

#### Remark valid for all Pu-Isotopes

For the sake of completeness it should further be mentioned that for <u>all</u> <u>Pu-isotopes</u> all f-factors larger than unity have now been set equal to unity also in order to avoid troubles upon the f-factor interpolation especially for high dilutions: In the MOXTOT-set a small number of f-factors with values slightly larger than unity appeared, mainly because of numerical reasons. They have been set equal to unity so that no further difficulties for an interpolation of the new f-factors are expected. This small modification, which was necessary only for some large  $\sigma$  -values, is considered to be of negligible importance for reactor calculations.

#### II.5 Sodium

Our data of sodium are based on the evaluation of SCHMIDT /6/. Since 1966 improved data have become available. In 1968 PITTERLE /56/ presented a new evaluation of the sodium data for ENDF/B. He made remarkable changes for the 2.85 keV resonance. The most important ones are the new width  $\Gamma_n$  and the new spin assignment J = 1 selected by PITTERLE. His revised  $\Gamma_{\gamma}$ -value is based on the result of FRIESENHAHN et.al. /57/. His changes for the values of  $\bar{\mu}(E)$  may also not be completely negligible for reactor calculations.

#### II.6 Oxygen

No recent measurements seem to be available for  $\sigma_{tot}$ ,  $\sigma_{el}$ ,  $\bar{\mu}_{el}$  of oxygen which cover the whole energy range of interest from 0.1 - 10 MeV or at least large parts of that range. Therefore we have not changed our group constants for this material.

However, it has been found that probably a minor inconsistency exists presently on the KEDAK-file which is also present in the SNEAK-set and the subsequent improved group-sets as e.g. MOXTOT-set or KFKINR-set. This has been concluded from the fact that above about 100 keV there is a variation in  $\bar{\mu}_{el}$  and even a change of sign between 160 and 170 keV, whereas  $\sigma_{el}$ , the elastic scattering cross section remains constant up to 270 keV.

#### II.7 Group Constants of the Thermal Group

In the documentation of the Russian ABN-set /58/ the group constants given in the thermal group (group 26) are the 2200 m/sec cross sections. Generally a Maxwellian weighting spectrum is applied, resulting in a multiplication of the 2200 m/sec values by the factor  $\sqrt{\pi}/2$ . When the SNEAK-set has been prepared /59, 60/ the weighting spectrum derived for the assembly SNEAK-3A2 has also been used to determine the group constants for the thermal group for those materials which are available on the KEDAK-file. Therefore in this set and in the subsequents sets, which are derived from the SNEAK-set, there exists an inconsistency in the thermal group (also in other groups, but there the importance is probably less pronounced): some materials having a Maxwellian weighting spectrum and the KEDAK-materials having the SNEAK-3A2weighting spectrum.

For some reactors, like STARK, where at least in some regions of the core an appreciable amount of neutrons is slowed down into the thermal energy range a Maxwellian weighting is more appropriate. Generally speaking, if the thermal group constants are important at all, a Maxwellian weighting is far more appropriate than the SNEAK-3A2-weighting spectrum. Therefore we replaced the thermal group constants by Maxwellian weighted 2200 m/secvalues for the KEDAK-materials and for some other materials where improved 2200 m/sec-cross sections were easily available.

We have used the evaluation of HANNA, WESTCOTT et.al. /36/ (H + W) and the KEDAK-data for the 2200 m/sec cross sections for  $\sigma_f$  and  $\sigma_c$  (see the following table)

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#### Origin of the 2200 m/sec-cross sections

Material	Al	С	Cr	Fe	Na	Ni
Data origin	KEDAK	KEDAK	KEDAK	KEDAK	KEDAK	KEDAK

Material	U235	U238	Pu239	Pu24o	Pu241	Pu242	U233
Data origin	H + W	KEDAK	H + W	KEDAK	H + W	KEDAK	H + W

For Pu239 a Maxwellian weighting may be not the best choice because of the possible influence of the resonance at about 0.3 eV on the group constants for the thermal group (0 - 0.215 eV). However, if the influence of this resonance really becomes important, the question of the weighting spectrum has to be considered more carefully and the group structure of the ABN-set will probably not be adequate enough in this case.

#### II.8 New Weighting Spectrum and Partial Anticipation of the REMO-Correction

For the SNEAK-set and the subsequent sets including the MOXTOT-set we have used the collision density of the assembly SNEAK-3A2 as weighting spectrum for the generation of group constants. This spectrum is similar to the spectrum of a steam cooled fast power reactor. It is more appropriate at present to use a spectrum which is typical of a sodium cooled fast power reactor. In addition we wanted to take into account - at least partially - in advance the effect of the REMO-correction which produces improved values for the elastic down scattering. Both items compare favourably well with the wishes of the industrial groups interested in the SNR-project: it will probably be possible to calculate a future SNR-type reactor without using the REMO-correction because the new weighting spectrum and the partial anticipation of the REMO-correction will lead to group constants for the elastic down-scattering which are reasonably well adapted to this special reactor type. For the industrial group this means a reduction of (a) computer time, (b) data handling, (c) necessary nuclear data files. An additional advantage for the calculation of reactor cells with the heterogeneity code ZERA /61/, /62/, for which the REMO-correction cannot be applied, consists in the fact that it will now be possible to use more appropriate group constants for the elastic down-scattering in this code too.

As new weighting spectrum we have chosen the collision density determined by a fundamental mode calculation for the central zone of the SNR using 208 energy groups. The following data have been used for this calculation:

Atomic densities  $(at/cm^3 \times 10^{24})$ 

u <sup>235</sup>	1.186-5	Fe	1.072-2
u <sup>238</sup>	4.732-3	Cr	3.163-3
Pu <sup>239</sup>	1.048-3	Ni	2.101-3
Pu <sup>240</sup>	3.073-4	0	1.228-2
241 Pu <sup>241</sup>	3.493-5	Na	1.057-2
Pu <sup>242</sup>	6.990-6	Мо	1.238-4
		Nb	9.834-5
		v	1.256-4

 $B^2 = 12.5 \cdot 10^{-4} \text{ cm}^{-2}$ , fuel temperature = 2100 °K

The resulting collision density integrals  $FI = \int F(E)dE = \int F(u)du$  $\Delta E_{\mathcal{B}} \qquad \Delta u_{\mathcal{B}}$ 

are given in <u>Table 1</u>. These results have been used to derive the collision density F(E) given in <u>Table 2</u>.

This collision density F(E) has been applied to generate new group constants for the elastic down scattering for the KEDAK-materials Al, C, Cr, Fe, H, Na, Ni, O, U235, U238, Pu239. In addition the collision density integrals FI have been used for the partial anticipation of the REMO-correction for the same materials with the exception of hydrogen. This has been done in order to minimize the effect of the REMO-correction for the SNR.

The partial anticipation of the REMO-correction (only applicable in the energy range above 1 keV, group 1 - 14) consists in a modification of the group constants for elastic down-scattering  $(\sigma_{be}^{\infty})$  for infinite dilution (background cross section  $\sigma_{o} \rightarrow \infty$ ). Some studies performed by Belgonucléaire have shown that for those materials in the SNR which are important for the elastic scattering process (namely Fe, 0, Na) the background cross section is generally about  $\sigma_{o} = 10$  barns. We have modified  $\sigma_{be}^{\infty}$  for each KEDAK-material in such a way, that the product  $\sigma_{be}^{\infty} \cdot f_{el}$  ( $\sigma_{o} = 10$  barns, T = 2100  $^{\circ}$ K) becomes equal to  $\sigma_{be}^{10}$  the corresponding value for the same material determined for the same background cross section by a slightly modified application of the usual REMO-correction using the SNR-collision density mentioned above.

$$\sigma_{\text{be},G}^{1o,I} = \frac{\int\limits_{E_{G}}^{E_{G-1}} \frac{\sigma_{el}^{I}(E) \cdot P_{el}^{I}(E \rightarrow E_{G}) \cdot F(E)}{\sigma_{tot}^{I}(E) + 10 \text{ barn}} dE}{\int\limits_{E_{G}}^{E_{G-1}} \frac{F(E)}{\sigma_{tot}^{I}(E) + 10 \text{ barn}} dE}$$

- F(E) = SNR-collision density
- $P_{el}^{I}(E) =$  probability that a neutron with energy E scattered on the isotope I will suffer an energy loss so that the final energy will be lower than  $E_{cl}$ .

In Fig. 1 - 3 is shown  $\sigma_{be}^{eff}(\sigma_{o})$  the effective microscopic group constants for elastic down scattering (SBE) as a function of the background cross section  $\sigma_{o}$ . The results obtained by an application of the REMO-correction are compared with the results obtained by the usual direct calculation using the so-called GROUCO-concept. In these cases we have still used the SNEAK-3A2-collision

density as weighting function both for the GROUCO- and REMO-calculation. In <u>Fig. 1 - 3</u> are shown some rather extreme examples to indicate the magnitude of possible discrepancies which may occure if the REMOcorrection is not taken into account. The materials considered and the group numbers according to the ABN-group-structure are given in the figures.

Some preliminary studies showed that the above modification was not completely sufficient. The main reason is that the real background cross section is not a constant within one group as is assumed for the corresponding formula given above for  $\sigma_{be}^{10}$ . In the REMO-procedure the group constant for the elastic down-scattering is determined in the following way

$$\sigma_{be,G}^{\text{REMO,I}} = \frac{\int\limits_{E_{G}}^{E_{G-1}} \frac{\sigma_{el}^{I}(E) P_{el}^{I}(E \rightarrow E_{G}) \cdot F(E)}{\Sigma_{tot}(E)} dE}{\int\limits_{E_{G}}^{E_{G-1}} \frac{F(E)}{\Sigma_{tot}(E)} dE}$$

If the total cross section of the composition  $\Sigma_t(E)$  is split up into the components of individual isotopes, we get

 $\Sigma_{tot}(E) = N_{I} \cdot \sigma_{tot}^{I}(E) + S_{J \neq I} N_{J} \cdot \sigma_{tot}^{J}(E)$ =  $N_{I}(\sigma_{tot}^{I}(E) + \sigma_{o}^{I,Rest}(E))$ where  $\sigma_{o}^{I,Rest}(E) = S_{J \neq I} \frac{N_{J}}{N_{I}} \cdot \sigma_{tot}^{J}(E)$ I, J = isotope index I = Index of one specific isotope considered

In <u>Fig.4</u> the collision density F(u) as function of the lethargy u is given for the composition of the central zone of the SNR. It shows rather large variations even within one coarse group of the Russian ABN group structure. This variation is taken into account appropriately for the determination of the elastic removal group constants of our new set of group constants. Fig. 5 shows the total macroscopic cross section for the composition of the central zone of the SNR. In Fig. 6 - 8 the same total cross section and the contributions of the components oxygen, sodium and iron, respectively, are given, whereas in Fig. 9 - 11 the total cross section and the total cross section without the components of oxygen, sodium and iron, respectively, are shown. From Fig. 5 - 11 it can clearly be seen that  $\Sigma_{tot}$  (E) and the background cross section  $\sigma_{1,\text{Rest}}^{I,\text{Rest}}(E)$  show appreciable variations within one coarse group. The fact that  $\sigma_{0}^{I,\text{Rest}}(E)$  is not constant within one coarse group has rather severe implications on the determination of the correct group constant for the elastic removal: the real range of integration in the numerator of the above expression is considerably smaller than from E<sub>G</sub> to E<sub>G-1</sub> as indicated in the formula; it is from E<sub>G</sub> to E<sub>G</sub>/ $\alpha^{I}$  where  $\alpha^{I} = ((A-1)/(A+1))^{2}$  and A is the atomic weight of the isotope I.

For the numerator of the above expression for  $\sigma_{be,G}^{\text{REMO},I}$  only that part of  $\sum_{tot} (E)$  and  $\sigma_{o}^{I,\text{Rest}}(E)$ , respectively, are relevant which are within the narrow range of integration just mentioned. For the denominator, however,  $\sum_{tot} (E)$  and  $\sigma_{o}^{I,\text{Rest}}(E)$  are relevant within the whole energy range from  $E_{G}$  to  $E_{G-1}$ . Because of the energy dependence of  $\sigma_{o}^{I,\text{Rest}}(E)$  within one coarse group this means that for a precise adjustment of  $\sigma_{be}^{\infty}$  the determination of  $\sigma_{be}^{10}$  is not sufficient in all cases because one would have to use instead of one background cross section, (e.g. 10 barns), as done for  $\sigma_{be}^{10}$ . The determination of such average values for the background cross section in the numerator and the denominator of an expression analogous to that given for  $\sigma_{be}^{10}$ . The determination of  $\sigma_{0,G}^{I,\text{Rest}}$  (denominator) or the equivalent, more elaborated determination of  $\sigma_{0,G}^{REMO,I}$  using the subsequent modification of  $\sigma_{be}^{\infty}$  for all groups and materials would also probably have been too specific to the central zone of the SNR to an extent which is not really necessary and probably too specific, we adjustments which are not really necessary and probably too specific, we adjusted only a few values of  $\sigma_{be}^{\infty}$  for the three isotopes oxygen, sodium and iron which are important for the elastic down-scattering in the SNR-

composition. The values used for the adjustment have been derived from calculated values of  $\sigma_{be,G}^{\text{REMO},\text{I}}$  for the three isotopes in some energy groups using in the REMO-procedure the collision density F(E) and total cross section  $\Sigma_{\text{tot}}(E)$  of the composition of the central zone of the SNR. This adjustment has been performed in those cases where it has found to be necessary in addition to the preceding adjustment of  $\sigma_{be}^{\infty}$  via  $\sigma_{be}^{10}$  for the following energy groups

group	oxygen	sodium	iron
6	_	yes	yes
7	yes		yes
8	_	_	
9	-	-	_
10	yes	yes	yes
11	-	_	yes
12	_	yes	yes
13 yes		yes	yes
14	yes	yes	yes

When applying the new group constants for elastic down-scattering generated with the new weighting spectrum and partially anticipating the REMO-correction one should be aware of the following effects:

 The SNR-collision density is typical of a relatively "hard" neutron spectrum. For reactors with "softer" neutron spectra, like those of the SNEAK-3-series /63/, /64/, these group constants are less suitable. This deficiency can only partially be removed (namely for the energy range above 1 keV) by the application of the REMO-correction.

- 2. The material composition of the SNR contains relatively large amounts of Na, Fe, O. The resonances of theses materials appreciably influence the collision density which is subsequently used as weighting function. If the amount of one or more of these materials is changed considerably (e.g. by changing sodium density, kind of structural material, kind of fuel) the collision density will also be changed so that the SNRcollision density may no longer be appropriate in this case.
- 3. As already indicated, the partial anticipation of the REMO-correction causes of modification or adjustment of  $\sigma_{be}^{\infty}$ . Therefore this value has no longer a physical meaning by itself.
- 4. The adjustment of  $\sigma_{be}^{eff}$  could only be performed for one special value of the background cross section (namely  $\sigma_{o}$  = 10 barns). If for some other compositions considerably different values of  $\sigma_{o}$  occur the effect of the adjustment will be reduced i.e. the agreement between the directly calculated effective group constants (using the adjusted  $\sigma_{be}^{\infty}$ -values) and the corresponding values determined by an application of the REMO-correction will generally be deteriorated. For large  $\sigma_{o}$ -values this deficiency is probably less severe because the material will be of minor importance for that special composition as indicated by its large dilution (high background cross section  $\sigma_{o}$ ). For the study of sodium-void-effects or for the determination of  $\sigma_{be}^{eff}$  for essentially pure materials, as e.g. a nickel-reflector, the mentioned deficiency has to be kept in mind. In those cases the effect of the REMO-correction generally will no longer be negligible.
- 5. Future changes of the presently established set of group constants have to take into account that changes in the resonance-selfshielding factors  $f_{el}$  have to be transformed into corresponding changes in  $\sigma_{be}^{\infty}$ . This means that  $\sigma_{be}^{\infty}$  has to be readjusted in order to preserve the merits of the present partial anticipation of the REMO-correction.

#### II.9 Special Weighting Spectrum for Carbon and Hydrogen (C1/Eo, H1/Eo)

It has been mentioned in the preceding paragraph that the presently used weighting spectrum (collision density for the inner core zone of the SNR) is not very suitable for the calculation of reactors with rather "soft" neutron spectra. Most times such kind of reactors contain rather large amounts of carbon and/or hydrogen in order to soften the neutron spectrum. In the extreme case of a very soft neutron spectrum the collision density will show approximately a 1/E dependence over a large energy range. Therefore we have used as an alternative weighting spectrum the following collision density:

$$F(E) = \begin{cases} \frac{2}{\Theta} \sqrt{\frac{E}{\pi\Theta}} \exp(-E/\Theta) \text{ with } \Theta = 1.41 \text{ MeV for } 2.5 \text{ MeV} \le E \le 10.5 \text{ MeV groups } 1 - 3 \\ C/E \text{ with } C = 0.4525 \text{ for } 0.215 \text{ eV} \le E \le 2.5 \text{ MeV (groups } 4 - 25) \end{cases}$$

In the high energy range this corresponds to the fission neutron spectrum for thermal fission of Pu239 (Maxwellian with a temperature of 1.41 MeV). Below 2.5 MeV we assumed a 1/E dependence as in the ABN-set; the constant C has been chosen so that at the high energy boundary (2.5 MeV) there is a continuous transition to the Maxwell-distribution.

In order to be able to study at least roughly the possible influence of a different weighting spectrum on calculated integral parameters as e.g. criticality or reaction rates we used this alternative weighting spectrum to generate modified group constants for carbon and hydrogen in addition to the group constants for the same materials which have been determined with the usual SNR-weighting spectrum. In order to distinguish them from the usual group constants we have used new labels: C1/E0 and H1/E0 respectively.

For carbon we replaced only the group constants for elastic down-scattering in groups 1 - 25; group 26 remains unchanged. It should be mentioned that in groups 1 - 14 the partial anticipation of the REMO-correction mentioned in the preceding paragraph has already been included using of course also the alternative weighting spectrum for the determination of the REMOcorrected group constants for elastic down-scattering needed for the adjustment. For hydrogen the alternative weighting spectrum has been used for the determination of all types of group constants in groups 1 - 25. The group constants for group 26 remained unchanged in this case too.

#### II.10 Fission Neutron Spectra

In a previous report /65/ the influence of fission neutron spectra on integral nuclear quantities of fast reactors has been studied. It has been shown that it is important to take into account the differences in the spectra of the various isotopes. It may also be important in some cases to take into account the variation in the fission neutron spectrum caused by a variation in the energy of the fission-inducing neutron. At the moment only the dependence on the isotope will be considered. Taking into account the dependence on the energy of the fission-inducing neutron would imply considerable modifications of the programs used for the calculation of the neutron distributions and is probably less important than the first effect. Therefore it we be disregarded at present.

We have decided to represent all fission spectra by Maxwellian distributions although this may not be justified for very low and very high energies. But the fission spectra in these energy ranges are not very important for fast reactor calculations because there are only a small number of neutrons in these energy ranges. In the important energy range a Maxwellian fit to the experimental results for the fission neutron spectrum measurements seems to be reasonable and until now no final conclusion has been reached which kind of representation (WATT-form or sum of Maxwell-distributions) should be used instead of Maxwell-form. The different temperatures T for the Maxwellian distributions for the various isotopes are given in the following table:

Isotope	Pu239	Pu240	Pu241	Pu242	Th232	U233	U234	U235	U236	U238
T [MeV]	1.41	1.39	1.34	1.39	1.32	1.31	1.31	1.30	1.31	1.35

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#### III. FIRST RESULTS FOR THE RECALCULATION OF FAST ZERO-POWER REACTORS

Some results of the preliminary version of the KFKINR-set have already been published /66/. The essential feature was that the absolute magnitude of the discrepancy between the calculated and measured criticality value is smaller than 1 % for all assemblies used in the preceding studies /66/, /8/ with one exception where the difference is 1.1 %. For the reaction rate ratios the agreement between theory and experiment was still not completely satisfactory. But it may be possible that the rather large discrepancies are due to errors in the experiments or in their evaluation and are not caused exclusively or primarily by errors in the nuclear data. For the steam density coefficient of criticality for the SNEAK-3A-series we had for the first time obtained an acceptable agreement between theory and experiment.

# III.1 Effect of the Partial Anticipation of the REMO-Correction on the <u>Calculation of the SNR</u>

One of the objectives of the KFKINR-set was to reduce the effect of the REMO-correction for the SNR-composition. This has been done

- (a) by using the collision density of a 208 group calculation for the central zone of the SNR as weighting function for the determination of the group constants for elastic down-scattering
- (b) by the partial anticipation of the REMO-correction as described before.

The fact that the anticipation of the REMO-correction is not done rigorously but treated only in an approximative manner, for reasons explained before, leads to be necessity that the success of the procedure has to be checked by a rigorous application of the REMO-correction to the specific SNR composition. In order to do this two ways are possible:

(I) using the collision density F(u) given by the 208-group calculation

(II) using the collision density obtained by the usually applied iterative procedure which consists in a smoothing of the collision density obtained by 26 group calculation and the subsequent use of the smoothed function for the determination of improved group constants

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for the elastic down scattering which are then used in the following 26 group calculation.

First we study the remaining effect of the REMO-correction on criticality. The following table gives the criticality difference for the MOXTOT- and KFKINR-set of group constants caused by the application the REMO-correction for the central zone of the SNR

	$\Delta \mathbf{k}$ (REMO)			
	MOXTOT-Set	KFKINR-Set		
REMO with 208-gr. F(u)	+0.0066	+0.0013		
REMO with iterative F(u)	+0.0058	+0.0002		

Δk(	REMO	) for	SNR

The remaining criticality difference of about 0.1 % can be considered as sufficiently small.

Next we study for the SNR the corresponding effect on the group constants SBE for elastic down scattering and on the energy dependence of the neutron flux  $\phi$ . The results of the conventional GROUCO-method without any REMO-correction are compared in <u>Fig. 12</u> (SBE) and <u>Fig. 13</u> ( $\phi$ ) with the results obtained when the REMO-correction is applied using the 208-group SNR-collision density. For the MOXTOT-set the differences are rather large:  $\pm$  50 % for SBE and up to 70 % for  $\phi$  whereas for the KFKINR-set the partial anticipation of the REMO-correction proves to be successful: the differences are smaller than about 5 % for SBE as well as for  $\phi$ . For the energy range below 1 keV which is outside the energy range of the REMO-correction, but may be important for the determination of the Doppler-coefficient, the KFKINR-set shows excellent agreement whereas the MOXTOT-set underestimates the flux by about 10 %.

It was interesting for us to see what results can be obtained by the application of the usual iterative treatment of the REMO-correction for the special case of the SNR-composition. In Fig. 14 and Fig. 15 the results for SBE and for

the neutron flux  $\phi$ , respectively, obtained by the iterative procedure and the conventional GROUCO-concept are compared with the corresponding results obtained by the application of the REMO-correction using the 208-group collision density. From these figures it can be seen that for the KFKINR-Set due to the partial anticipation of the REMO-correction, which means an adjustment of  $\sigma_{be}^{\infty}$  as described before, the iterative procedure deteriorates to some extent the rather satisfactory results obtained with the conventional GROUCO-concept for the SNR composition. This concerns also the energy range below 1 keV which is outside the range of the REMO-correction but is affected by the effect of the REMO-correction on the group constants for elastic down-scattering for energies above 1 keV. In the upper part of Fig. 14 and 15 the corresponding results for the MOXTOT-set are also shown. The results for both sets of group constants, KFKINR and MOXTOT, are very similar. This is probably caused by the fact that for both sets of group constants the smoothed curves for the collision density used in the iterative procedure differ in a characteristic and consistent manner from the corresponding curve obtained by a 208-group calculation. Fig. 16 and 17 give a comparison of the 208-group collision density with the collision density determined by the iterative procedure using the KFKINR-Set. These figures demonstrate that due to the influence of resonances of predominantly scattering materials, as e.g. oxygen, sodium, and iron, the 208-group collision density shows a rather marked structure within one coarse group which naturally can not be found in the smoothed curve derived from 26-group results. Above about 2 MeV the deviations of the two curves in Fig. 16 and 17 may partially be caused by the fact that in the 208 group calculation the energy distribution of the fission neutrons can be taken into account more appropriately than in the 26-group calculation.

In order to avoid any misinterpretation of the results presented before it should be stressed that the good agreement between the results obtained with the conventional GROUCO-concept and those obtained by an application of the REMO-correction using the 208-group collision density is only valid for the composition of the central zone of the SNR. For compositions with similar amounts of coolant, structural material, and oxide fuel, as e.g. the blanket of the SNR, it is expected that the agreement will not be much worse than for the central zone of the SNR. For compositions with appreciable

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differences (a) in the amounts of the materials (e.g. coolant loss) or (b) in the kind of the materials (e.g. carbide fuel) compared to the SNR-composition the above conclusions are no longer applicable. The conventional GROUCO-concept will no longer be sufficient and the REMO-correction has to be applied. Comparing the results for the MOXTOT-set shown in the upper parts of <u>Fig. 14</u> and 15 (iterative REMO-procedure) with those shown in the upper parts of <u>Fig. 12 and 13</u> (conventional GROUCO-concept) gives some indication that for those compositions which differ markedly from the SNR-composition the iterative REMO-procedure will produce results which will be considerably improved compared to those obtained by the conventional GROUCO-concept. From <u>Fig. 16</u> and 17 we conclude that, although the iterative treatment of the REMOcorrection provides a good first approximation for the desired quantities (as e.g. SBE, neutron flux  $\phi$ ), it is preferable to use for each specific composition considered the corresponding 208-group collision density if it is already available or can easily be obtained.

The conclusions of this chapter with respect to the KFKINR-set can be summarized as follows

- (I) For the SNR the effect of the REMO-correction on the criticality and on the neutron flux in 26 group-calculations is sufficiently small.
- (II) For the SNR the usual iterative treatment of the REMO-correction deteriorates to some extent the rather satisfactory results obtained with the conventional GROUCO-concept.
- (III) For compositions which differ appreciably in the components of its materials from the SNR composition the REMO-correction can no longer been omitted.
- (IV) If the REMO-correction has to be applied it seems preferable to use - if easily available - the 208-group collision density for the corresponding mixture; otherwise the usual iterative procedure should be used.

#### III.2 Criticality of Specific Fast Assemblies

In order to check the new set of group constants we recalculated the values of the criticality for some specific fast assemblies. We have chosen essentially the same assemblies as already used before /8/, /67/ for checking nuclear data and methods of calculation. Some results especially for the S<sub>N</sub>-correction and for the influence of taking into account the P1-approximation for the neutron scattering on hydrogen for the assembly SUAK-UH1B have been taken from the preceding reports /8/ and /67/. Other criticality corrections e.g. heterogeneity-, REMO- and fission spectrum-corrections have been redetermined using the new KFKINR-set. The influence of the fission spectrum on criticality has been described in a separate report /65/. The fission spectrum correction listed in Table 3 has been determined usually by fundamental mode diffusion calculations-except for SNEAK-3B2 were a one-dimensional diffusion calculation has been performed.

In order to determine the fission spectrum correction we started with the pure fission spectrum of the main fissionable isotope, i.e. U235 and Pu239 respectively, and then take into account appropriately the contributions of other isotopes, e.g. U238, to the fission spectrum of the material composition considered. The basic values for  $k_{eff}$  in <u>Table 3</u> have been obtained in different ways for the various assemblies: (a) by fundamental mode diffusion calculations (b) by one- or two-dimensional transport calculations (c) by two-dimensional diffusion calculations.

The fission spectrum corresponding to the basic  $k_{eff}$ -values is indicated in a separate column of <u>Table 3</u>. Generally we have used the SNR-collision density as weighting spectrum for the generation of the group constants for the elastic down-scattering. For assemblies with rather soft neutron spectra as e.g. SNEAK-5C it seems more appropriate to use also a softer weighting spectrum. Therefore we used in those cases a weighting spectrum which is essentially a 1/E collision density as explained before in chapter II.9. The weighting spectrum used for each assembly is also indicated in a extra column of <u>Table 3</u>. The heterogeneity correction has been determined as usually by an application of the ZERA-code to the heterogeneous and quasihomogeneous case.

In <u>Table 4</u> the criticality values obtained with different sets of group constants are compared with the experimental results for the different assemblies. For most of the assemblies studied the criticality value obtained with the final KFKINR-set differs by an amount of less than 1 % from the experimental results. This is also true for the assemblies labelled SNEAK-3A-series given in Table 3. Only three out of the about fifteen assemblies are outside the ± 1 % region of criticality differences:

ZPRIII-55:  $\Delta k = \pm 1.1 \%$ . This difference is only slightly larger than the 1 % margin; furtheron it should be mentioned that the heterogeneity correction depends to some extent on the weighting-spectrum (WS): for the SNR-WS it is 1.5 %, for the 1/E-WS 1.2 %. A more precise determination of the heterogeneity correction which would require the application of the appropriate weighting spectrum may probably bring the criticality difference for this assembly below the 1 % margin.

For SUAK-UH1B the reasons for the criticality difference  $\Delta k = -2.0 \%$  are not yet clear. Two possible explanations seem to be near at hand: (I) Some specific group constants in the high energy range (E > 2 MeV) of particular high importance for this assembly may still be somewhat erroneous.

(II) It may be necessary to take into account the higher moments of the angular distribution of the elastic scattering, i.e. P1, P3 or P5, instead of the transport-approximation which is used up to now. Apart from effects which are important for similar assemblies too, as e.g. SUAK-U1B, the higher moments for the elastic scattering on hydrogen and carbon may be important for SUAK-UH1B. The effect of taking into account the P1-approximation for the scattering on hydrogen has been studied before /67/. In addition to the criticality correction  $\Delta k \approx +0.003$ derived from one-dimensional transport calculations which is quoted in /67/ it is probably worthwhile to mention that in fundamental mode calculations with 26 and 208 energy groups we have obtained a criticality difference of +0.007 to +0.008 when we used the P1-approximation for the scattering on hydrogen instead of the transport approximation. In the fundamental mode calculations the buckling has been kept constant when changing from the transport- to the P1-approximation. The value of about +0.007 is close to the originally /68/ given value. The difference to the probably more reliable value of +0.003 determined in /67/ indicates that the spatial flux shape is changed appreciably by the transition from the transport-
to the P1-approximation for the scattering on hydrogen. Further studies must show if the P1-approximation for the scattering on hydrogen and the transport-approximation for the scattering on carbon are sufficient for a precise determination of the criticality and the spatial flux shape for the assembly SUAK-UH1B.

The assembly SNEAK-5C is a rather extreme case within the framework of the present study because of its "soft" neutron spectrum leading to a median fission energy of about 1 keV. The criticality difference to the experiment of +2.1 % given in <u>Table 4</u> may partially be caused by the fact that neither the SNR- nor the 1/E-weighting spectrum seem to be sufficiently appropriate to this special assembly. The heterogeneity correction for SNEAK-5C shows a remarkably large effect of the weighting spectrum:  $\Delta k_{het} = +0.066$  for the 1/E-WS and  $\Delta k_{het} = +0.075$  for the SNR-WS. The large magnitude of the heterogeneity correction give rise to some doubt wether the code and its inherent assumptions and approximations are accurate enough to guarantee reliable results even in this extreme case.

<u>Table 4</u> shows that the value for the root mean square deviation  $\sqrt{(\Delta k)^2}$  for the final KFKINR-set is somewhat worse than for the preliminary version of the KFKINR-set. This is mainly due to the two assemblies SNEAK-5C and SUAK-UH1B discussed just before, which show criticality deviations of about 2 % for the final KFKINR-set. If we would omit these two assemblies the root mean square deviation would decrease from 0.0097 to 0.0055 while the average criticality deviation  $\overline{\Delta k}$  would remain nearly unchanged.

The check of the KFKINR-set of group constants has been extended to other assemblies which were not considered in the preceding study /8/. For SNEAK-6A and SEFOR-1C the criticality difference is within the 1 % margin generally observed (this statement also holds for the MOXTOTresults for both assemblies). For some other assemblies listed in the following table the comparison of the experimental criticality values with the corresponding calculated values using the MOXTOT- and the new KFKINR-set shows that by the preparation of the KFKINR-set the criticality prediction has generally been improved and that now similar criticality values have been obtained for classes of similar assemblies.

	k eff			
ASSEMBLY	EXPERIMENT	MOXTOT-Set	KFKINR-Set	
zebra-8h	1.027	0.996	1.022	
ZPRIX-25	1.000	0.975	0.995	
SNEAK-2A-R1	1.000	1.029	1.013	
SNEAK-6A-Z1	1.000	1.000	1.007	
GODIVA	1.000	1.016	1.0108	
JEZEBEL CLEAN Pu	1.000	1.000	1.0114	
JEZEBEL DIRTY Pu	1.000	0.997	1.0091	
VERA-11A	1.000	1.000	1.0064	

k<sub>eff</sub>-values for some additional assemblies

		Basic k value eff	Fission spectrum used	Weighting spectrum used	$s_N^{-}$ correction	Heterogeneity correction	REMO- correction	Fission spectrum correction	Other corrections	Best available <sup>k</sup> eff
SUAK U	1B	0.8513	U235	SNR	-		-0.0002	+0.0012	-	0.8523
SUAK U	H1B	0.9211	U235	SNR	_	+0.0017	-0.0010	+0.0004	+0.0030 (2)	0.9252
ZPRIII	-10	0.9753	U235	SNR	+0.0127	+0.0105	+0.0007	+0.0013	-	1.0005
ZPRIII	-25	0.9863	U235	SNR	+0.0023	+0.0085	+0.0004	+0.0023	-	0.9998
ZPRIII	-48	0.9852	<sup>°</sup> Pu239	SNR	+0.0077(1)	+0.0140	+0.0002	-0.0006	_	1.0065
ZPRIII	-48B	0.9843	Pu239	SNR	+0.0077	+0.0140	+0.0002	-0.0006	-	1.0056
ZEBRA-	6 <b>a</b>	0.9873	Pu239	SNR	+0.0115		-0.0006	-0.0005	-	0.9977
(4)	(-3Ao	0.9255	U235	SNR	+0.00384	-0.0008	-0.0009	+0.0003	-	0.9315
SNEAK	-3A1	0.9545	U235	SNR	+0.0038	+0.0009	°o.	+0.0003	· _	0.9631
Series	-3A2	0.9895	U235	SNR	+0.0043	+0.0024	≈0.	+0.0002	- - 	1.0000 <sup>(3)</sup>
	(-3A3	1.0324	U235	SNR	+0.0043	+0.0060	-0.0003	+0.0002	-	1.0462
SNEAK-	3A 1	0.9985	U235	SNR	+0.0038	+0.0009	~o.	+0.0003	· -	1.0035
SNEAK-	3A2	0.9939	U235	SNR	+0.0043	+0.0024	≈0.	+0.0002	-	1.0008
SNEAK-	3B2	0.9997	Pu239	SNR	+0.0043	+0.0030	+0.0011	-0.0035	_	1.0046
ZPRIII	-55	0.9980	Pu239	SNR	-	+0.0149	+0.0009	-0.0026	_	1.0112
SNEAK-	5C	0.9928	Pu239	1/E	_	+0.0663	-0.0069	-0.0002		1.0520

<u>Table 3:</u> Basic k eff values, criticality corrections and best available k eff the KFKINR-set of group constants

(1) The correction determined for one assembly is also applied to the other assembly

(2) Effect of using the P1-approximation for the scattering on hydrogen instead of the transport approximation

(3) The  $k_{eff}$  -values for the SNEAK-3A-Series are normalized to  $k_{eff}$  (SNEAK-3A2) = 1.0

(4) The experimental k -values are: 3Ao: 0.930, 3A1: 0.962, 3A2: 1.000 (normalization), 3A3: 1.048

ω1

	······						
	<sup>k</sup> eff						
ASSEMBLY	EXPERIMENT	SNEAK- Set	MOXTOT- Set	preliminary KFKINR-Set	final KFKINR-Set		
SUAK U1B	0.86 ± 0.01	0.855	0.856	0.859	0.852		
SUAK UH1B	0.945 ± 0.01	0.918	0.930	0.940	0.925		
ZPRIII-10	1.	0.999	1.011	1.002	1.001		
ZPRIII-25	1.	0.980	0.998	0.989	1.000		
ZPRIII-48	1.	0.977	0.989	0.995	1.007		
ZPRIII-48B	1.	0.975	0.987	0.997	1.006		
zebra-6a	1.	0.974	0.985	0.991	0.998		
SNEAK-3A1	1.	0.994	1.019	1.007	1.004		
SNEAK-3A2	1.	0.989	1.012	1.006	1.001		
SNEAK-3B2	1.	0.984	0.998	0.997	1.005		
ZPRIII-55	1.	0.958	0.984	0.991	1.011		
SNEAK-5C	1.031 ± 0.005	1.026	1.042	1.028	1.052		
<u></u> (1)		-0.0173	-0.0022	-0.0033	+0.0020		

Table 4: Measured and calculated criticality values for various fast assemblies and different sets of group constants

(1) 
$$\overline{\Delta k} = \frac{1}{N} \sum_{i=1}^{N} \Delta k_i$$
, (2)  $\sqrt{(\Delta k)^2} = \sqrt{\frac{1}{N}} \sum_{i=1}^{N} (\Delta k_i)^2$ 

(2)

 $(\Delta k)^2$ 

 $\Delta k_{i} = k_{eff}$ , calculated-k<sub>eff</sub>, measured for assembly i

0.0270

0.0062

0.0125

0.0097

#### III.3 Influence of the Weighting Spectrum on Criticality

For the generation of group constants for two materials, namely carbon and hydrogen, we have used in addition to the usual SNR-weighting spectrum a different, rather "soft" weighting spectrum, which is essentially a 1/E collision density. The influence of this difference in the weighting spectra has been studied for a few assemblies where rather large effects had been expected. The results of fundamental mode diffusion calculations are listed below. Besides the results without the application of the REMOcorrection, the last column also shows the criticality differences obtained when the REMO-correction is used in both cases: calculations using group constants for C and H with the SNR-WS and with the 1/E WS.

	Results wit	orrection	Δk	
ASSEMBLY	k <sub>eff</sub> with SNR-WS	k eff with 1/E-WS	Δk	with REMO-correction
ZPRIII-55	0.9954	1.0156	+0.0202	+0.0033
SNEAK-5C	0.9779	0.9916	+0.0137	-0.0071
HECTOR HUG	1.0822	0.9861	-0.0961	-0.0930
HECTOR HPG	1.0494	0.9739	-0.0755	-0.0801

Criticality effect of different weighting spectra

As expected the effects are very pronounced for the HECTOR-HUG and - HPG experiments. In these experiments homogenized mixtures of graphite with fissile material (uranium for HUG, plutonium for HPG) have been used for  $k_{\infty}$ -experiments. Because of the very "soft" neutron spectra - the median fission energy is about 100 eV - the inclusion of the REMO-correction which applies only above 1 keV brings about no large additional effect for the criticality differences. For ZPRIII-55 and SNEAK-5C the different weighting spectra lead to considerably smaller criticality differences than obtained for the HECTOR experiments. For SNEAK-5C with a median fission energy of about 1 keV the application of the REMO-correction leads to a change of sign for the criticality difference compared to the value obtained by using directly the different weighting spectra. The

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remaining criticality difference  $\Delta k \approx -0.7 \%$  is still considerably large and indicates that the energy range below 1 keV which can not be treated at present by our code for the REMO-correction is of some importance for the determination of the criticality. For ZPRIII-55 with a median fission energy of about 150 keV the application of the REMO-correction reduces the criticality difference by an appreciable amount compared to the value determined by using directly the group constants generated for the two weighting spectra. The remaining criticality difference of about 0.3 \% may not be totally due to differences in the group constants for elastic down-scattering below 1 keV but may also partially be caused by the fact that above 1 keV the corresponding REMO-corrected group constants which are obtained by starting from "SNR-weighted" and "1/E-weighted" group constants respectively still show some small differences.

## III.4 Results for Reaction Rate Ratios

We have studied here as in /66/ essentially three reaction rate ratios  $F^{8}/F^{5}$ ,  $C^{8}/F^{5}$ ,  $F^{9}/F^{5}$  where F and C mean fission and capture, respectively, and 8, 5, 9 stand for U238, U235, Pu239, respectively. The  $F^8/F^5$  ratio is now generally overestimated by about 8 % compared to the experimental results with the exception of SNEAK-3A2 where the underestimation by about 20 % is probably caused by an erroneous experimental result.  ${\rm C}^8/{\rm F}^5$  is slightly underestimated (about 3 %) and  $F^{9}/F^{5}$  is predicted even better (discrepancies of about 1 %). The larger underprediction of about 10 % for  $F^{9}/F^{5}$  in ZPRIII-55 is probably caused to a large extent by difficulties in the interpretation of the complicated procedure adopted in order to obtain the experimental result (see also /69/). For SNEAK-5C the interpretation of the experimental results especially for  $C^{8}/F^{5}$ and  $F^{9}/F^{5}$  is complicated by the strong influence of heterogeneity effects and by the fact that neither the SNR- nor the 1/E-weighting seem to be appropriate for the recalculation of this experiment. Furtheron for  $F^9/F^5$  a new experimental technique has been applied for the first time so that a systematical error cannnot be excluded for the experimental result.

We recalculated some reaction rate ratios which were measured recently in SNEAK-6D. The ratio of calculated to experimental results for different sets of group constants is listed below.

	MOXTOT-Set	Preliminary KFKINR-Set	KFKINR-Set
c <sup>8</sup> /F <sup>5</sup>	1.01	1.07	1.05
F <sup>8</sup> /F <sup>5</sup>	0.87	0.91	0.99
F <sup>9</sup> /F <sup>5</sup>	0.91	0.95	0.98
c <sup>8</sup> /F <sup>8</sup>	1.17	1.18	1.07
c <sup>8</sup> /F <sup>9</sup>	1.11	1.12	1.07

Reaction Rate Ratios for SNEAK-6D Theory/Experiment

The improvement obtained with the KFKINR-set is obvious. The remaining discrepancy is concerned with the capture rate in U238. The theoretical results are 5 - 7 % higher than the experimental ones. This fact is somewhat surprising because for other assemblies a slight underestimation has been found as mentioned above. One possible explanation for this contradictory behaviour is that the standard used for the evaluation of the more recent experiments is due to some doubts: some deviation has been observed between the standards used by two different groups of experimentalists operating at the STARK- and SNEAK-facility, respectively. It will not be possible to draw more definite conclusions on the correctness of the theoretical results for the capture rate in U238 determined with the KFKINR-set until the presently existing discrepancy of the experimental standards has been removed in the measurements.

#### IV. SUMMARY

The most important changes in the new group constants compared to those of the MOXTOT-set, which was the reference set, concern the fuel isotopes of fast reactors, namely U235, U238, Pu239, and Pu240. For the less pronounced but still important changes we must refer to the detailed description given in chapter II. Some of the more remarkable changes will be briefly indicated in the following. For U235 we have reduced the  $\alpha$ -values below 1 keV  $(\alpha = \sigma_c / \sigma_f)$  by a considerable amount. For the capture cross section of U238 we have tried to use group constants which are - together with those for the fission cross section of U235 - consistent with differential measurements of the cross section ratio  $\sigma_{c}(U238)/\sigma_{f}(U235)$ . For U238 we have reduced the group constants for inelastic scattering and changed the inelastic scattering probabilities in such a way that the spectra of the inelastically scattered neutrons are shifted towards higher energies. For Pu239 our new group constants are based to a large extent on the recent Karlsruhe evaluation performed by Miss HINKELMANN /37/. Our group constants for the total cross section of U235, U238, and Pu239 have been modified in accordance with the recent measurements of CABE et.al. /1/. We have found that for accurate calculation and evaluation it is essential to use fission spectra which are different for the different fuel isotopes.

The new group set - KFKINR - has three special features differing from the preceding MOXTOT-set: (I) the group constants in the thermal group have been determined using a Maxwellian spectrum as the weighting function, (II) for the generation of the group constants for elastic down-scattering of the materials available on KEDAK, namely Al, C, Cr, Fe, H, Na, Ni, O, U235, U238, and Pu239 we have used the collision density of the central zone of the SNR as the weighting function and, in addition, partially anticipated the usual REMO-correction. (III) In order to be able to calculate, at least approximately, the nuclear characteristics of assemblies with rather "soft" neutron spectra, we have determined additional sets of group constants for C and H for which the collision density used as the weighting function was composed of a fission neutron spectrum (above 2.5 MeV) and a 1/E-spectrum (between 0.215 eV and 2.5 MeV).

As a first check we confirmed that, because of the partial anticipation of the REMO-correction, the effect of the exact treatment of the REMO-correction on criticality, group constants for elastic down-scattering and energy dependence of the neutron flux is sufficiently small for the central zone of the SNR so that the REMO-correction may be omitted for routine-calculations of the SNR. Generally we have observed that the difference between calculated and measured criticality-values is within a  $\pm$  1 % uncertainty range. For the two remarkable exceptions, it seems likely that the methods of calculation presently used are not refined enough, so that the larger criticality difference observed in these two cases can not certainly be attributed to errors in the group constants only.

With respect to reaction rate ratios it has been shown that with the KFKINR-set the experimental results, especially for a more recent SNR-mock-up in SNEAK, can now be calculated rather well with the exception of the capture rate in U238, where the agreement is not completely satisfactory. But in this special case the experimental difficulties seem to be not completely resolved in the integral measurements in critical assemblies and the differential measurements of the capture cross section give rise to some uncertainty too.

The first test-calculation have shown that the presently available KFKINR-set of group constants provides a firm basis for the design calculations of sodium cooled fast power reactors. Further checks with experimental results obtained in critical facilities like SNEAK, STEK, SUAK, STARK, ZPR-III, ZPR-VI, ZPR-IX. ZPPR, ZEBRA and MASURCA will hopefully confirm this experience, increase the confidence level indicate directions of possible further improvements, especially with respect to the presently not so highly important materials as e.g. structural materials or fission products.

# V. APPENDIX: REMARKS ON THE METHODS OF CALCULATION

A) Studies on the validity of the assumption of additivity of the S<sub>N</sub>-corrections for different space directions.

Most of the assemblies studied here and practically all power reactors of interest can be treated at least approximately by two-dimensional calculations in cylindrical (r,z)-geometry. These calculations are most times done using diffusion codes, because two-dimensional transport codes need much computer time and are sometimes not easily available. The use of the 2d-diffusion codes instead of the more appropriate 2d-transport codes comprises a certain approximation with respect to the angular dependence of the neutron flux and the leakage of neutrons. This approximation influences to some extent the criticality parameter determined in the calculations. The criticality difference between transport- and diffusion-calculations is called  $S_N$ -correction. The exact determination of the  $S_N$ -correction would require two- or three-dimensional transport calculations which are very time-consuming and sometimes impossible since the corresponding codes are not available or even not yet existing. Instead of the exact  $S_N$ -correction one uses sometimes an approximate value which is obtained by adding up the  $S_N$ -corrections determined in one-dimensional calculations e.g. in r- and z-direction.

This procedure would be correct if the assumption of the separability of the spatial neutron flux distribution would be valid. Therefore the assumption that by adding up the one-dimensional  $S_N$ -corrections of the r- and z-direction one is able to obtain the correct two-dimensional  $S_N$ -correction is equivalent to the assumption of the spatial separability of the neutron flux.

An alternative procedure consists in establishing an "equivalent" spherical model of the cylindrical reactor, e.g. by using a so-called shape factor, and determining by one-dimensional calculations for this spherical model the magnitude of the  $S_N$ -correction which is then assumed to be the same for the real cylindrical configuration. Both procedures can only provide approximate values for the  $S_N$ -correction and it seemed interesting to us to study the validity of these procedures in a few specific cases.

As a first check we considered one of the SUAK assemblies, namely SUAK U1B. The SUAK assemblies are exceptions in our present study because they have cubic geometry instead of the usual cylindrical geometry. For most of the cylindrical assemblies, studied in this work, the assumption of the separability of the flux shape in the different space directions has been verified /8/ by means of two-dimensional diffusion calculations in cylindrical geometry and comparison of the criticality value with corresponding one-dimensional diffusion theory results. For the determination of the energy-independent bucklings used in the one-dimensional calculations the usual iterative procedure has been applied which is outlined in /8/ p. 17. The analogue procedure has been used in the case of SUAK U1B where we performed a two-dimensional diffusion calcu-

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lation in x-y-geometry using an energy-independent buckling for the z-direction which has been determined in the usual manner and has been taken in the onedimensional calculations too.

For the assembly SUAK U1B we obtained the following results of the diffusion calculations with the SNEAK-set, using  $B_z^2 = 58.2967 \cdot 10^{-4} \text{ cm}^{-2}$ ;  $k_{eff}(2 \text{ dim.}) = 0.82368 \pm 0.0004$ ,  $k_{eff}(1 \text{ dim.}) = 0.82375 \pm 0.0001$ . The difference between both values is smaller than 0.0001 which is well within the accuracy of both calculations. This means that the present comparison indicates that for the SUAK-assemblies too the assumption of the separability of the flux shape in the x- and y-space directions seems to be fairly well realized.

During our previous study /8/ only a one-dimensional  $S_N^{-}$ code was available at Karlsruhe. We determined the total transport correction by adding up the  $S_N^{-}$ correction of the different space directions. We are now able to check the validity of the assumption of the additivity of the  $S_N^{-}$ corrections by means of a two-dimensional  $S_N^{-}$ code called SNOW. Because the effect of the additivity-assumption was most pronounced for the SUAK assemblies, the first (see /8/, tables V-15g and V-15h) check has been done for SUAK U1B for which we have shown just before that the assumption of separability of the flux shape in the different space directions holds reasonably well.

The results for the one-dimensional  ${\rm S}_{_{\rm N}}\text{-}{\rm corrections}$  were the following ones:

x-direction:  $\Delta k_{SN,x} = 0.0087$ y-direction:  $\Delta k_{SN,y} = 0.0087$ z-direction:  $\Delta k_{SN,z} = 0.0139$ 

resulting in a total SN-correction of  $\Delta k_{SN,total} = 0.0313$ . For the spherical model of this assembly, described in detail in /8/, we have obtained  $\Delta k_{SN,sphere} = 0.013$  which was considerably smaller than the  $\Delta k_{SN,total}$  given above. This difference illustrates the importance of the assumption of the additivity of the one-dimensional SN-corrections. The reason for this difference is most probably due to an inadequate boundary condition in the diffusion calculation for the spherical model as discussed in more detail in /8/ page 56. The result of a two-dimensional S<sub>4</sub>-calculation in x-y-geometry, which was confirmed by a corresponding S<sub>8</sub>-calculation, yielded a criticality

value which was larger by an amount of 0.0173 than the corresponding diffusion theory calculation. This criticality difference agrees with the corresponding sum of the one-dimensional  $S_N$ -corrections ( $\Delta k_{SN,x}$  +  $\Delta k_{SN,y}$  = 0.0174) within the accuracy of the calculations and is definitely larger than the one-dimensional  $S_N$ -correction for the sphere  $\Delta k_{SN,sphere}$  = 0.013. The results of these calculations verify the validity of the assumption of the additivity of the  $S_N$ -correction at least for those assemblies of our previous study /8/ for which this assumption is most important, namely for the SUAK-assemblies. But one must have in mind that the SUAK-assemblies have the special feature that they have no reflector regions in the x- and y-directions. Therefore the above mentioned conclusion may not be applicable for small reflected assemblies.

For the other assemblies of our previous study /8/ the effect of the assumption of the addivity of the  $S_N$ -correction is less pronounced than for the SUAK-assemblies just mentioned: with the exception of the SUAK-assemblies the largest criticality deviation between the  $S_N$ -correction for the spherical model and that obtained by adding up the  $S_N$ -correction in radial and axial direction is 0.0016 (see /8/ table V-15c). This is a rather small amount compared to other possible sources of errors which may be involved in the determination of the criticality. If one wants to study the validity of the above mentioned assumption in such cases one must be quite sure that the programs used for this kind of study are reliable and the results are accurate enough to draw definite conclusions. Especially the influence of the mesh size and the influence of the convergence criteria for the accuracy of the eigenvalue, the source and the flux on the calculated criticality value should be precisely known.

Another example for which both, the  $S_N$ -correction itself and the difference between the results of both approximate procedures of determining the  $S_N$ -correction were reasonably large was the assembly VERA-11A which was not considered in /8/. Therefore we performed a similar study for this assembly as was outlined before for SUAK U1B.

For the spherical model we adjusted the radius of the core in such a way that we obtained in the one-dimensional diffusion calculation the same criticality value as in the two-dimensional diffusion calculation. The specifications used for the one- and two-dimensional models are given in <u>Table A1</u>. From one-

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dimensional transport- and diffusion-calculations we obtained for the spherical model a transport correction  $\Delta k_{SN,sphere} = + 0.0468$ . For the alternative procedure, i.e. adding the transport corrections of the separated axial and radial directions, we obtained a total  $S_N$ -correction of  $\Delta k_{SN,total} = \Delta k_{SN,ax} + \Delta k_{SN,rad} = + 0.0558$ . The correct two-dimensional transport correction of + 0.0483 lies in between of the results of the two alternative one-dimensional procedures. However, for VERA-11A, the assembly considered here, the result for the spherical model is closer to the correct result than that obtained under the assumption of the additivity of the  $S_N$ -corrections for the separated space directions.

Probably this fact can not be generalized to other assemblies of different configurations, because for the specific example of VERA-11A

- (a) the height to diameter ratio of 0.8 is close to unity so that the spherical model is a fairly good representation of the real cylindrical configuration and
- (b) the axial and radial reflectors are of extra ordinary importance for the leakage and consequently for the criticality of the assembly too.

As is well known the assumption of separability of the flux becomes poor in the blankets and this may be the reason why the resulting transport correction  $\Delta k_{SN,total} = \Delta k_{SN,ax} + \Delta k_{SN,rad}$  is not in too good agreement with the correct result. For other cylindrical assemblies where the assumption of separability is better fulfilled than for VERA-11A, the transport correction  $\Delta k_{SN,total}$  may be closer to the correct two-dimensional transport correction than that determined for a spherical model.

B) Studies with the two-dimensional transport code SNOW for the assembly
<u>VERA-11A</u>

The two-dimensional transport  $(S_N)$ -code SNOW has been developed at Karlsruhe. At the beginning of its use for production runs only little experience from the test runs was available with respect to choosing reasonable values for the mesh-size (h) and the angular resolution (N). It seemed useful to study the dependence of the criticality on both parameters at least for one assembly. We haven choosen VERA-11A for that purpose because this assembly has a rather small cylindrical core but was reflected in both radial and axial direction by rather thick uranium reflectors. Therefore this assembly seemed to be suitable for a two-dimensional transport code: the transport correction should be large and the separation of the space-dependence (where the radial and axial direction are treated separately by a one-dimensional transport code using the buckling concept) becomes doubtful because the large reflectors in both directions are of considerable importance for the space-dependence of the neutron flux and for the criticality parameter so that in this case the separation-ansatz may become a poor approximation.

First we studied the influence of the mesh size on the criticality. The results are given in <u>Fig. A1</u>. The mesh sizes in radial  $(h_r)$  and axial  $(h_z)$  direction are normalized to the energy-averaged transport mean free path  $(\overline{\lambda}_{tr} \approx 3.11 \text{ cm} \text{ for VERA-11A})$ . We found that it was convenient in drawing this figure to show the dependence of the criticality on the product of  $(h_r/\overline{\lambda}_{tr}) \approx (h_z/\overline{\lambda}_{tr})$ . No further thoughts have been given to the observation of a nearly linear dependence for reasonably small mesh sizes. From <u>Fig. A1</u> it can be concluded that for this assembly the following relations are valid:

for  $h \approx \overline{\lambda}_{tr}$  criticality is underestimated by less than 0.2 % for  $h \approx 1/2 \cdot \overline{\lambda}_{tr}$  criticality is underestimated by less than 0.05 % for  $h \approx 1/3 \cdot \lambda_{tr}$  criticality is underestimated by less than 0.02 %

From <u>Fig. A1</u> it can also be seen that 11 energy groups are sufficient if an accuracy of 0.1 % is required. From the 4 group-results it must be concluded, that probably even the  $S_8$ -approximation is not sufficient for the special case considered here, because the criticality-difference between  $S_h$  and  $S_8$  is larger than 0.2 %.

Therefore we studied in more detail the influence of the angular resolution on the criticality. The results are given in <u>Fig. A2</u>. Trying to extrapolate from S<sub>2</sub>, S<sub>4</sub>, S<sub>6</sub>, S<sub>8</sub> - the highest angular resolution which is presently allowed in the code - to S<sub>w</sub> we arrived at <u>Fig. A3</u>. The approximately linear dependence of the criticality on N<sup>-3</sup>, N being the order of the S<sub>N</sub>-calculation, shown in <u>Fig. A3</u> may be as fortuitous as that observed in <u>Fig. A1</u> for the dependence of the criticality on the product  $(h_r/\bar{\lambda}_{tr})$   $(h_z/\bar{\lambda}_{tr})$ . If extrapolation is justified in <u>Fig. A3</u> we would conclude that, compared to S<sub>w</sub>; the S<sub>6</sub>-result overestimates the criticality by less than 0.1 % for this assembly and the S<sub>8</sub>-result by less than 0.05 %.

Mixture Material	1	2
C	460.6	
Cr	15.8	16.8
Cu	79.6	-
Fe	60.7	64.6
Ni	6.65	7.1
Pu239	72.4	-
Pu24o	3.7	-
U235	_	2.5
U238	-	344.0

Table	<u>A1</u> :	CRITICAL	ASSEME	BLY:	VERA-	-11A <sup>(</sup> *)	1)
;		Atom-Dens	sities	(in	1020	atoms/	-m <sup>3</sup> )

### Fundamental Mode Calculation:

NG	MIXT	BUCK.
26	1	174.6263.10 <sup>-4</sup> cm <sup>-2</sup>

- (\*) Most of the data presented here have been taken from W.J. PATERSON and J.W. WEALE: J. Brit. Nucl. Energy Soc. 3, p. 311, October 1964 and from A.R. BAKER: ANL-7320, p. 116, 1966. The core radius resp. blanket thickness for the spherical case has been determined, respectively guessed by ourselves.
  - 1) The abbreviations used here are the same those in /8/

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GEØ	NG	BUCKLING	BC	NZ	NP
SLAB	26	110.0.10 <sup>-4</sup> cm <sup>-2</sup>	23	3	101

# One-Dimensional Calculations:

ZONE IZ	MIXT	XL [cm]	INT	XR [cm]
1	1	0.	10	5.0
2	1	5.0	10	10.8712
3	2	10.8712	80	52.07

GEØ	NG	BUCKLING	BC	NZ	NP
CIT	26	$58.0.10^{-4}$ cm <sup>-2</sup>	23	3	127

ZONE IZ	MIXT	XL [cm]	INT	XR [cm]
1	1	0.	10	5.0
2	1	5.0 26		13.4747
3	2	13.4747	· 90	58.42

GEØ	NG	BUCKLING	BC	NZ	NP
SPHERE	26	-	23	3	115

ZONE IZ	MIXT	XL [cm]	INT	XR [cm]
1	1	0.	10	50
2	1	5.0	18	14.1556
3	2	14.1556	86	57.1556

Two-Dimensional Diffusion Calculations

GEO	NG	NP	ROWS	C	DL	NZ	BCI	Ľ,	BCR	BCUI	2	BCLOW	SPE	ECTRUM F	OR COND
2	- 11	1440	36		+0	5	2		3	3		2	1-c	lim. SPH	ERE
NEW (	GROUP	<u> </u>	1	2	3	4	5	6	7	8	9	10	11		
IGUP	OLD (	ROUP	3	4	5	6	7	8	9	10	12	16	26	· · · ·	n North Contraction

MIXT	I	II	III
MIXTURE	1	1	2
PHI-1 dim (IZ)	1	2	3

Zone	MIXT	RL [cm]	INTH	RR [cm]	HUP [cm]	INTV	HLOW [cm]
1	I	0.	5	4.0	4.0	5	0.
2	II	4.0	13	13.4747	10.8712	16	0.
3	II	0.	5	4.0	10.8712	11	4.0
4	III	13.4747	21	58.42	52.07	35	0.
5	III	0.	18	13.4747	52.07	.19	10.8712

Two-Dimensional Transport Calculations

GEO	NG	NP	ROWS	COL	NZ	BCL	BCR	BCUP	BCLOW	SPECTRUM FOR COND
2	11 26	1326	34	39	5	2	3	3	2	1-dim SPHERE (Diff.)

NEW GROUP	1	2	3	4	5	6	7	8	9	10	11
IGUP OLD GROUP	3	4	5	6	7	8	9	10	12	16	26

MIXT	I	II	III
MIXTURE	1	1	2
PHI-1 dim (IZ)	1	2	3

ZONE	MIXT	RL [cm]	INTH	RR [cm]	HUP [cm]	INTV	HLOW [cm]
1	Ţ	0.	2	4.0	4.0	2	0.
2	II	4.0	6	13.4747	10.8712	6	0.
3	II	0.	2	4.0	10.8712	4	4.0
4	III	13.4747	30	58.42	52.07	33	0.
5	III	0.	8	13.4747	52.07	27	10.8712

For our new set of group constants we have used the SNR-collision density as weighting spectrum for the generation of the group constants for elastic downscattering. The REMO-correction has been applied in order to take into account the fact that the correct collision density of each reactor considered here differs from the SNR-collision density. An intrinsic feature of the procedure applied to determine the REMO-corrections consists in the smoothing of the collision density which is obtained as a step function in 26-group-calculations. This smoothing process is performed mainly under mathematical aspects; in general, from the point of view of neutron physics it does not improve the information which is contained in the 26-group results nor does it provide any additional information. It allows to take into account the coarse shape of the collision density but it is not able to take notice of the fine structure which would be present in the exact collision density (i.e. in a fine-group or ultrafine-group representation) due to the influence of resonances of the fuel-, coolant- and structural-material (e.g. oxygen, sodium and iron). Consequently there remains a certain amount of inaccuracy in the determination of the group constants for elastic down-scattering, even if the REMO-correction is applied. The effect of this uncertainty on the criticality has been studied by using the fine-group representation of the collision density obtained in 208-group fundamental mode calculations for each assembly. Besides the individual collision density of each assembly we have used two reference collision densities:

- (I) the SNR-collision density
- (II) a collision density F(u) = constant, which is independent of the lethargy u.

With each of these collision densities we collapsed the 208-group constants to 26-group constants and performed 26-group fundamental mode calculations. The criticality differences obtained between the values obtained by using the individual collision density of the assembly and the collision densities (I) and (II), respectively, are given in <u>Table A2</u>. The criticality differences given in <u>Table A2</u> provide a certain indication of the amount to which the weighting spectrum may influence the calculated criticality value (here of course not only because of its influence on the group constants for elastic down-scattering but also because of its influence on the other types of group constants, i.e. capture, fission, inelastic, transport etc). The large criticality differences observed in <u>Table A2</u> result primarily from shifts of the neutron spectrum which are caused essentially by differences in the 26-group constants for elastic down-scattering, determined by collapsing with different collision densities.

For comparison the results of the usual REMO-correction are given in <u>Table A2</u> too. Comparing both results one must, however, have in mind that:

- (a) the REMO-correction is determined for the whole assembly, whereas the other results are determined for fundamental mode calculations only.
- (b) the criticality differences obtained by group collapsing with different collision densities result from the influence of the weighting spectrum on all types of group constants, not only on those for elastic downscattering as is the case for the REMO-correction.

Comparing the first and third column of <u>Table A2</u> one finds that in general the results are similar. One major discrepancy occurs for ZPRIII-25. This may be caused by the fact that the group constants (scattering matrix) for inelastic scattering are not changed by the REMO-procedure, in contrast to the case of group collapsing with different collision densities. The inelastic scattering has proved to be of high importance for the criticality of the assembly ZPRIII-25.

The first and third column of <u>Table A2</u> show that in 26-group calculations including the REMO-correction the uncertainty of the criticality parameter due to inaccuracies of the weighting spectrum will in general be smaller than about 0.005.

The second column of <u>Table A2</u> shows that the weighting spectrum should not be too crude because otherwise the uncertainties in the calculated criticality values become too large. In this case also the accuracy of the calculated neutron spectrum will probably not be sufficient for the comparison with experimental results.

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Assembly	k(individual collision density)	k(individual collision density)	k(with REMO-correction) -k(KFKINR-Set with SNR- collision-density
	-k(SNR-collision density)	-k(constant collision density)	weighting spectrum for elastic slowing down group constants)
SUAK U1B	-0.0001	-0.0025	-0.0002
SUAK UH1B	-0.0008	-0.0019	-0.0010
ZPRIII-10	+0.0019	-0.0012	+0.0007
ZPRIII-25	+0.0056	+0.0003	+0.0004
ZPRIII-48	+0.0018	-0.0090	+0.0002
zebra-6a	+0.0023	-0.0076	-0.0006
(3Ao	-0.0040	-0.0086	-0.0009
SNEAK- 3A1	-0.0024	-0.0067	≈0.
Series 3A2	-0.0016	-0.0052	≈o.
3A3	-0.0012	-0.0038	-0.0003
SNEAK 3A1	-0.0020	-0.0066	≈o.
SNEAK 3A2	-0.0016	-0.0052	~o.
ZPRIII-55	-0.0002	-0.0260	+0.0009
SNEAK-5C	+0.0088	-0.0161	{+0.0139 -0.0069 <sup>(x)</sup>
HECTOR HUG	-0.0071	-0.0018	an an Arran an Arra an
HECTOR HPG	-0.0012	-0.0060	
VERA-11A	-0.0037	-0.0016	
GODIVA	-0.0029	-0.0034	
zebra-8h	+0.0054	-0.0020	
ZPRIX-25	+0.0046	-0.0026	

Table A2: Criticality differences obtained by group collapsing from 208 to26 groups using different collision densities as weighting function

 $(\mathbf{x})$ Here C1/Eo has been used for carbon in the KFKINR-Set

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2.667578E-06	3.630155E-06	4.731338E-06	6.004750E-06	7.477667E-06
9.235254E-06	1.133091E-05	1.379890E-05	1.662664E-05	2.002930E-05
2.406561E-05	2.925446E-05	3.462068E-05	4.044331E-05	4.723543E-05
5.477574E-05	6.239965E-05	7.152118E-05	8.209891E-05	9.234445E-05
1.007177E-04	1.116019E-04	1.208020E-04	1.309169E-04	1.413016E-04
1.515392E-04	1.689568E-04	1.800059E-04	1.801338E-04	1.893594E-04
2.023653E-04	2.205890E-04	2.506571E-04	2.682335E-04	2.847007E-04
3.026426E-04	3.154548E-04	3.258991E-04	3.494646E-04	3.744038E-04
3.900961E-04	3.932740E-04	4.919581E-04	5.130924E-04	5.177665E-04
4.991845E-04	5.143094E-04	5.313533E-04	5.416994E-04	5.429790E-04
5.692458E-04	5.858466E-04	5.726316E-04	6.234844E-04	6.432042E-04
6.775139E-04	7.133896E-04	7.560435E-04	7.864940E-04	7.742003E-04
7.482877E-04	7.572284E-04	7.803978E-04	8.053959E-04	8.059689E-04
8.130430E-04	8.094083E-04	9.142100E-04	1.073779E-03	1.257944E-03
1.665756E-03	1.746941E-03	1.830400E-03	1.743142E-03	1.679684E-03
1+821869E-03	1.884392E-03	1.978656E-03	2.131557E-03	2.266697E-03
2.398586E-03	2.275567E-03	2.081119E-03	1.905396E-03	1.806709E-03
1.876689E-03	2.069107E-03	2.107218E-03	2.240751E-03	2.321616E-03
2.241935E-03	2.389244E-03	2.532790E-03	2.359786E-03	2.418477E-03
2.488333E-03	2.563050E-03	2.503411E-03	2.550427E-03	2.893760E-03
2.781094E-03	2.656971E-03	2.775204E-03	2.710670E-03	2.683517E-03
3.010913E-03	2.717097E-03	2.593298E-03	2.519039E-03	2.434739E-03
2.482473E-03	2.518213E-03	2.825721E-03	2.918712E-03	2.815591E-03
2.908966E-03	3.005836E-03	2.553707E-03	2.806577E-03	2.510507E-03
2.660277E-03	2.458631E-03	2.202567E-03	2.121033E-03	2.360429E-03
2.586300E-03	2.450741E-03	2.261385E-03	2.261287E-03	2.259893E-03
2.233175E-03	2.204790E-03	2.203887E-03	2.210624E-03	2.278948E-03
2.591324E-03	2.752052E-03	2.066668E-03	1.697372E-03	1.716414E-03
1.698581E-03	1.680393E-03	1.645638E-03	1.632875E-03	1.633707E-03
1.646120E-03	1.767604E-03	1.680154E-03	1.498800E-03	1.441064E-03
1.463667E-03	1.410644E-03	1.297613E-03	1.237310E-03	1.205264E-03
1.171157E-03	1.138414E-03	1.123905E-03	1.130359E-03	1.136298E-03
1.142415E-03	1.127025E-03	1.040772E-03	9.640623E-04	9.270350E-04
9.049408E-04	8.599006E-04	8.043007E-04	7.824318E-04	7.549508E-04
7.193075E-04	6.879256E-04	6.361534E-04	5.444307E-04	4.660599E-04
4.505890E-04	4.485378E-04	4.443182E-04	4.577169E-04	4.809753E-04
5.088826E-04	5.390628E-04	5.569721E-04	5.730200E-04	5.820827E-04
5.826245E-04	5.750207E-04	5.619079E-04	5.482070E-04	5.285351E-04
5.081252E-04	4.845306E-04	4,558426E-04	4.042664E-04	3.676382E-04
3.482667E-04	2.506473E-03	7.876386E-04	2.135969E-04	2.826528E-05
4.429258E-06	4.059760E-07	3.623187E-08	1.082072E-08	1.079714E-09
5.259511E-11	1.117080E-12	8.349990E-15		

Table 1

208-group collision density integrals

$$FI_{g} = \int_{\Delta Eg} F(E) dE = \int_{\Delta ug} F(u) du$$

for the central zone of the SNR beginning with g = 1 at the high energy end

C.C		0.0	0.9215777E	04	0.2324065E-05
C.1(7500CE	CO	0.38E3717E-13	0.9733867E	C4	0.22644515-05
C.3399999	00	C.4468318E-11	C. 1028099E	65	0-2201663E-05
(.7324995F	00	C-9620869E-10	0.1085877F	05	0.2186128E-05
0.15749985	01	C.9358827F-09	0.1146901F	05	0.22500955-05
C.3300007F	cī.	0.43:828FF-18	A. 12113855	05	0.2210440E-05
1.7204CC5E	61	C. 6772212E CO	0.12704325	05	0.20605005-05
C 1576CC0E	6.2	0.25202255-07	A 1261226	02	0.2020200245-05
C 3300004E	02	0.35302276-01	Uel321332E	02	0.20290346-03
0.7226066	C 2		0.15074005	02	0.21335295-05
U. 15249748	02		U.100/489E	ଏ 🗩 -	0.2100085-05
C.13/3000E	03		-0.19922085	0.0	0.18913425-05
0-33664485	63	0.31505538-05	0.15816885	05	0.17772016-05
C.7324998E	03	0.46849948-05	C.1776196E	05	0.16817895-05
C.1028099E	04	0.6197054E-C5	0.1876016E	05	0.1604747E-05
C.1CE5E77E	64	0.6193683E-C5	C.1981446E	05	0.1551451E-05
C.11469C2E	04	C.6448387E-05	C.2692800E	05	0.1484752E-05
C.1211356E	64	0.6884166E-C5	0.2210894E	05	0.1409328E-05
C.1279433E	Ç4	C.6928098E-05	C.2336133E	05	0.1318978E-05
C.1351335E	C4	0.68788555-05	0.2468466E	05	0.1519852E-05
C.1427278E	C4	C.6774456E-C5	0.26082965	05	0.1915390E-05
C.1507489E	64	0.6652727E-05	0.2756046E	05	0.17068435-05
C.15922C8E	C4	0.6456155E-C5	0.2912166E	05	0.1420616E-05
(.1681688E	64	C.6255285E-C5	0.3077129E	05	0.1304150E-05
C. 1776197E	C4	0.6000771E-05	C. 3251436E	05	0.1230474E-05
C.1876016E	C4	C.5676185E-C5	C.3435618E	05	0.1164984F-05
0.1981446E	64	0-52505025-05	0.3630233E	05	0-11167265-05
C.2002801F	04	0.4F69712F-05	1.3835871E	05	0-10695035-05
0.10108655	64	0.4436181E-(5	0.40531505	65	0.10127915-05
C. 22241245	64 64	0 30543745-(5	C. 49977555	0.5	0.05953745-04
C 24464475	0-4 6 A	0 35371605-05	0 452521995	0 J 6 S	0.92000192-00
0 24004070	64	0.31054675-65	009223371E 0 17009056	00	0.00025025-06
U . 20002300	07 04		0.50404455	02	0,90733735-00
0 201000400	0-2		V.2V47403C	0.2	0.000000010-00
0.29121000	U4 01	0.27560212-03	V•222333335	02	
0.30771295	04		U. 3033100E	02	0.71505362-06
(.3231436E	04	0.20021085-05	U. 3444842E	02	0.135/0962-06
0.34356188	04	0.2876713E-05	0.62843275	05	0.1741695E-06
C.3630233E	04	0.31811612-05	C.6637606E	05	0.6917044E-06
C.3835872E	C4	0.32556385-05	0.7010756E	05	0.7321185E-06
0.40531588	04	0.3221699E-C5	C.7404881E	<b>Ç</b> 5	0.6306907E-06
C.4282750E	C4	0.32000025-05	0.7821169E	05	0.7028522E-06
C.4525352E	C4	0.31387015-05	0.8260856E	05	0.6439860E-06
0.47806995	C4	0.3076775E-05	C.8725263E	05	0.5901467E-06
(.5(45457E	04	0.3114391E-C5	0.9215775E	05	0.57919555-06
C.5333328E	C4	0.3103013E-05	0.9733863E	05	0.5308947E-06
C.5633156E	04	0.3009623E-05	0.1025378E	60	0.4961383E-06
C.5949836E	04	0.2963246E-(5	0.10774228	06	0.46546535-06
C.6284320E	04	0.3028766E-05	0.1132109E	06	0.4344643E-06
C. 6637609E	04	C.3105184E-C5	0.1189571E	66	0.4277985E-06
C.701C762E	C4	0.2980069E-05	C.1249949E	06	0.4191314E-06
(.74C4887F	04	0.2806349E-05	C.1313393F	60	0.4179263E-06
(.7821172F	04	0.2643074E-15	0.1380056F	06	0.4407516F-06
0.8260855F	04	C.2488126F-05	C. 1450103F	06	0-37384965-06
C.8725266E	04	0.2386102E-05	0.1523705F	66	0.3593890E-06
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Table 2

Collision density F(E) for the central zone of the SNR

C.1601044E	60	0.3501723E-06	0.1758518E	07	0.7817267E-08
C.1682308E	06	0.31905978-06	C.1832977E	07	0.7153965E-08
C. 1767696F	06	0-31783465-06	C.1910381F	07	0.6847504F-08
(.1857418E	66	C-2147335E-C6	C. 1991162E	07	0-64443175-08
C. 1CF1ACAE	ñĂ	n_26200105-06	0.20753595	07	0.59845145-08
C 20803545	СС С С С	0 24450045-04	A. 2142114E	67	0.55720725-00
C - 21542455	04	0 0/0000000000	A 33246046	07	0 55457025-00
1021246425 1 00240165	00	0 3310120020-04	V 22 37 307 C	07	0 57729135-00
0 22301430	10 A4		C 24402945	- ∿ / ∧ 7	0.00272013C-VC
0.23731420	00	0.10000555-04	V.2997200E	07	0 44075415-00
Lo2433039E	UC 2/	0.15(09955-04	U=2042010C	07	00-30400700-00
1.20201000	00		V.ZCZ390/C	1. f 10 77	0 A1014155-00
	VO OV	U-1140/302-UO	U.Z/192020	101 A7	0.07000046.00
L.2900207E	00		0.28121012		0.37020345-08
0.30474115	00	0.13:90412-00	0.29081105	07	0.3330#12E=08
C.2202088E	60	C.14136775-C6	0.30073985	07	0.3124738E-08
0.33646155	06	0.1265215E-C6	0.3110075E	C7	0.28988485-08
C.35353915	66	C.1182325E-C6	0.32162588	07	0.2636972E-08
C.3714836E	60	C.1020574E-C6	C.3326066E	07	0.2402428E-08
C.3903389E	66	0.93505155-07	C. 3439623E	07	0.21708875-08
C.41C1512E	60	0.93849828-07	C.3557057E	07	0.1847402E-08
C.4309691E	60	0.9755331E-07	C.3678501E	07	0.1638824E-08
C.4528436E	6)	0.10151525-06	0.3804091E	07	0.14828695-08
C.4758284E	60	C.1C18348E-C6	0.39339695	07	0.1364051E-08
C.49997998	60	0.915864CE-C7	C.4070573E	07	0.1275281E-08
C.5253573E	06	0.8196594E-07	0.4214213E	07	0.1156209E-08
C.5520226E	60	C.72411C1E-C7	C.4362922E	07	0.1001660E-08
C.5800414E	06	0.65629995-07	C.4516879E	<b>C7</b>	0.9021595E-09
C.6054823E	66	C.6C38744E-C7	C.4676268E	07	0.8073715E-09
C.64C4176E	06	0.52585295-(7	0.48412815	07	0.71959515-09
C.6725231E	60	0.523087E-C7	0.50121185	07	0.6421357E-09
C.7(7C784E	06	0.5229610E-07	0.5188982E	67	0.5597574E-09
C.7429673E	60	C.475CC73E-C7	C.5372C89E	07	0.49572415-09
C.786778E	60	0.4310522E-C7	0.55616578	07	0.4257050E-09
C.E163127E	60	C.38556775-07	C.5757912E	07	0.3582168E-09
C.84960375	66	C.21622365-07	C.5961C94E	<u>C7</u>	0.30187795-09
C.8842524E	66	C.2586811E-07	0.6171446E	07	0.2559626E-09
C.9203142E	6	C.22C0528E-C7	C.6389221E	07	0.2132035E-09
C.9578467E	60	0.21237975-07	C.6613256E	07	0.1785436E-C9
C.5569057E	60	0.20228268-07	<b>C.6843720E</b>	07	0.1476923E-09
C.1037566E	07	0.1942204E-07	C.7082215E	07	0.1205977E-09
C.1(79875E	<b>C7</b>	6.18681505-07	0.73290215	07	0.9586670E-10
C.1123919E	C7	0.1685726E-07	0.7584427E	07	0.7710070E-10
C.1169755E	07	0.16005465-07	C.7848735E	C7	0.6184724E-10
C.1217460E	C7	0.1591105E-07	0.8122253E	(7	0.4960031E-10
C.1267110E	<b>C7</b>	C.1553016E-C7	C.8405302E	07	0.3935739E-10
C.1318786E	(7	0.14343725-07	0.8698215E	07	0.3099815E-10
C.137257CE	C7	0.1300429E - 07	0.9001336E	07	0.24253475-10
C.1429598E	C7	C.1144468E-C7	C. 9315021E	07	0.18820295-10
6.1490C49E	C7	0.10424362-07	0.9639637E	07	0.1432978E-10
C.1553056E	C7	0.96946815-(8	0.9975566E	07	0.10624365-10
C.1618727E	67	C.E542784E-C8	C.1032321E	08	0.7544283E-11
C.1687176E	07	0.83852895-08	0.1050000E	08	0.6299999E-11

Table 2 (continued)

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Fig. 2: Comparison of elastic removal constants using different calculational procedures
























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## Fig. A1

Influence of the mesh size on the criticality Studied for the assembly VERA-11A using the twodimensional transport code SNOW





Fig. A2

Influence of the angular resolution (N) on the criticality Studied for the assembly VERA-11 using the twodimensional transport code SNOW

## Fig. A3

Influence of the angular resolution (N) on the criticality Studied for the assembly VERA-11A using the twodimensional transport code SNOW



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