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Institut für Angewandte Systemtechnik und Reaktorphysik
Projekt Schneller Brüter

KAPER – Lattice Program for Heterogeneous Critical Facilities (User's Guide)

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by

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Abstract

This report is a documentation of the KAPER program, which is a multigroup lattice code developed to analyze experiments performed in plate-type heterogeneous critical facilities. Included in this documentation is a detailed description of the input data required for the program, the structure of the program, and an outline of the theoretical methods utilized in the program.

20.11.1973

KAPER - Zellprogramm für heterogene kritische Anordnungen

(Benutzer-Anleitung)

Zusammenfassung

Der vorliegende Bericht ist eine Dokumentation des KAPER-Programms, einem Multigruppen-Zellcode. Dieses Programm ermöglicht die Analyse von Messungen an heterogenen kritischen Anordnungen in Plattengeometrie. Der Bericht enthält eine genaue Beschreibung der für das Programm erforderlichen Eingabedaten, der Programmstruktur sowie der im Programm verwendeten theoretischen Methoden.

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KAPER - Lattice Program for Heterogeneous Critical Facilities

(User's Guide)

This report is to serve as a documentation of the KAPER program as it exists since January 1973. Included in this documentation is a detailed description of the input data required for the program, the structure of the program, and an outline of the theoretical methods utilized in the program.

The program was developed to function on the IBM/370 within the Karlsruhe NUSYS program system. However, the program can be easily used outside of the system without any internal changes in the code. In addition, sufficient details are given so that, for example, interfacing with other codes as multi-dimensional diffusion theory programs, can be performed.

The theoretical methods utilized are described in a reprint of a paper published in the proceedings of the conference on "Mathematical Models and Computational Techniques for the Analysis of Nuclear Systems". This paper is included in a section of this report and describes, among other things, a number of improvements which have been made in the program since the release of Ref. /1/. The most significant changes are the following:

1) A procedure for the calculation of anisotropic diffusion coefficient in the cell,

2) Fission source representation generalized to include individual fission spectra for all fissionable isotopes of the cell. This relaxes the assumption associated with a "universal fission spectrum".

The user of this program is requested to communicate to the authors any difficulties or errors associated with the use of the program and errors, or points needing greater clarification, in this documentation.

I. Introduction

The KAPER program is a dynamically dimensioned program in an overlay structure. The computer core space needed for the program is adjusted at the beginning of each calculation by specifing on the job control cards the amount of core space desired. The calculation of the space required for a problem is given in a section following the description of the input cards.

The three main segments of the KAPER program consist of the following:

A) phase for the calculation of heterogeneous resonance self-shielded cross sections in a multiregion cell,

B) phase for the calculation of the flux and adjoint distributions in the cell with associated reaction rates,

C) phase for the calculation of heterogeneous small-sample reactivity worths.

These segments overlay each other during the sequence of the calculation as given by the input cards. Information is passed to each segment by means of external units which are declared by job control cards.

At present the program considers only infinite plate geometry. No symmetry is assumed for the cell so that a cell specified in a calculation is assumed to be repeated infinitly in both directions.

II. Input Card Description

All data required on the following cards is entered format free. The convention is that the first parameter of an input card (labeled here as K4, for example) must begin in the first column of the card. The following parameters of the input card can be entired anywhere on the card, up to and including column 80, with a minimum of one blank space between parameters. Two or more cards may be used for the data of one input card (K). In the second and succeeding cards the first column of the card must be blank. All literal data required must be entered between alphas (α) or apostraples (').

1) Initiation of a series of KAPER calculations. The following three cards can be identical to those used in a NUSYS calculation of the Karlsruhe program system.

K1	αKAPERα	The field is free and can be used for identication of the job, as for example αNORMAL CORE CELL OF SNEAK-900Aα
K2	NFPH	Number of first phase for KAPER calculation; normally 99999.
K3	αENDEα	Constant

2) Phase 99999, Cross Section Phase. In this phase the resonance self-shielded cross sections for the heterogeneous cell are calculated and stored on external units for use in subsequent phases. While most calculations will be for a true heterogeneous

cell it is possible in this phase to prepare cross sections for a homogeneous medium. This is accomplished by specifying a two region cell with the same isotope mixture in each region. In addition, card K6 would contain NISS=1 and ISON(1)=αKEINEα. The resonance self-shielding is then calculated for the homogeneous composition as it is customarily performed in the program α00446α of the NUSYS system of Karlsruhe. To identify these cross sections as homogeneous (for other phases of the KAPER program), card K9 should contain NREG>1.

K1	α99999α	Constant
K2	(GRSN(I),I=1,3)	Group cross section set name (15 character name, e.g. α26-GR.KFKINR001α)
K3	NOG	Number of energy groups (≤26); see Section VII.
	NB	Number of terms (recommended NB=6) in the approximation of the reaction coefficients by a series of rational functions. (See explanation on card K4)
	KGEO	Free parameter, no meaning at present
	NFPH	Number of the following phase
	IH	5; Constant
	NOR	Number of isotopes for which reaction rates are to be calculated (NOR≤NIS of card K5). The cross section types SFISS (fission) and SCAPT (capture) are calculated, along with the cell cross sections, and are stored on unit NAP (see card K9) for the isotopes specified by IS(I) (see also card K9).

NCHI

a) If NCHI=0, the internal fission neutron spectra are used in all calculations.

b) For NCHI>0, specifies the number of fissionable isotopes for which a fission spectrum is read in as input (cards K10 and K11).

c) For NCHI<0, new fission neutron spectra, having a Maxwellian shape, are to be calculated for one of the following reasons:

1 - The energy group structure of the cross section set used is different than that of the Karlsruhe sets,

2 - The temperature of the fissionable isotopes is to be changed from that given internally in the program,

3 - A combination of 1 and 2.

Within KAPER are fission neutron spectra for the fissionable isotopes. These spectra have a Maxwellian shape,

$$\hat{\chi}^g = \int_{\Delta E_g} dE \; \frac{2}{T\sqrt{\pi T}} * \sqrt{E} \exp\left(-E/T\right)$$

where g is the energy group index. The temperatures (T) for the various isotopes, as given in KAPER, are:

^{232}Th = 1.32 MeV		^{233}U = 1.31 MeV	
^{234}U = 1.31 MeV		^{235}U = 1.30 MeV	
^{236}U = 1.31 MeV		^{238}U = 1.35 MeV	
^{239}Pu = 1.41 MeV		^{240}Pu = 1.39 MeV	
^{241}Pu = 1.34 MeV		^{242}Pu = 1.39 MeV	

The energy group structure of the spectra is that of the 26-groups in the Karlsruhe cross section sets (see Ref. /2/ and Section VII).

K4 GAM1 = 0.0
GAM2 = 30.0
GAM3 = 0.0
EBS1 = 0.02
EBS2 = 0.005

} Recommended values

These variables of card K4 are utilized in the calculation of the resonance self-shielding of the cross sections. The first three variables are used to define the fictitious background cross sections, b_i, in the approximation

$$\frac{P_{mn}\ (\sigma_{t\nu},\ \sigma_o)}{\sigma_{on} + \sigma_{t\nu}} \simeq \sum_{i=1}^{NB} \frac{a_i}{b_i + \sigma_{t\nu}}$$

(see Eq. (2.8) in Section VI.). NB is defined on card K3. The background cross sections are defined as

$$b_i = \langle \sigma_t \rangle * ALP^{(i-1)}$$

where $ALP = GAM1 + \left[GAM2 + GAM3 * \left\langle \sigma_t \right\rangle * \left\langle \frac{1}{\sigma_t} \right\rangle \right]^{2/(NB-1)}$

The last two variables on card K4 are used to test the degree of resonance self-shielding of the isotopes. In the energy groups in which the condition

$$\left| f_t(\sigma_o=o) - 1.0 \right| \leq EBS1$$

is satisfied, where $f_t(\sigma_o=o)$ is the total self-shielding factor for the fully self-shielded condition, the resonance self-shielding is handled as in the homogenized cell. For the case that the condition

$$\left| f_t(\sigma_o=o) - 1.0 \right| \leq EBS2$$

is satisfied the resonance self-shielding is completely neglected.

K5	NIS	Total number of isotopes (NIS≤20)
	(ISOT(I),I=1,NIS)	Isotope names as specified by the convention of the cross section set; e.g. αPU9A0α (5 character name). See Section VII for clarifications.
K6	NISS	Number of isotopes for which the influence of the cell structure on the resonance self-shielding of the cross sections is to be considered. The resonance self-shielding of all isotopes of card K5 which are not given again on card K6 is calculated as for a homogenized cell. (NISS≤NIS)

	(ISON(I),I=1,NISS)	Isotope names, e.g. αPU9AOα
K7	NR	Number of regions into which the cell is divided (NR≥2)
	(D(I),I=1,NR)	Thickness of the $i^{\underline{th}}$ region in cm
	(MIS(I),I=1,NR)	Mixture number of the $i^{\underline{th}}$ region as determined by the order in card K8.
K8	NMIS	Number of different mixtures
	((CON(J,I),I=1,NIS),J=1,NMIS)	Isotope concentration as $(atoms/cm^3)*10^{-24}$
K9	NREG	1; If the cross sections are being prepared for the calculation of fluxes of the normal core cell in phase 99998. 0; If the cross sections are being prepared for reactivity worth calculations or for the perturbed cell option in phase 99998. >1; If the cross sections are being prepared for a homogeneous flux calculation in phase 99998.
	NAP	External unit number on which cross sections are to be written for use in a succeeding phase. If NAP<0 a rewind is executed before writing, otherwise the unit

is held at the end of the last record written in a preceding phase 99999 calculation. In this manner the cross sections for reactivity worth samples can be stacked one after the other on the same unit. The space needed on this unit for each calculation can be determined from the equation for SPACE.

$$SPACE(words)=\lceil (5+NR)*NOG*NOR+(2+NOG)*NFI+NOG*NOG*NR+NR*NOG*(2+NFI)+4+NR+NWY \rceil$$

where NR = number of regions in the cell

NOG = number of energy groups

NFI = number of fissionable isotopes included in the isotope list of the problem

NOR = number of isotopes for reaction rate calculation

NWY = 0 if NREG=0
= (3+NR)*NR*NOG if NREG>0

(IS(I),I=1,NOR) Number of the isotope in the ISØT(I) array for which reaction rate cross sections are desired. If NOR=0 then the IS(I)'s are omitted.

S1 If NCHI=0, end of card input for phase 99999, otherwise go to K10 if NCHI>0 or to K12 if NCHI<0.

(Cards K10 and K11 are repeated NCHI times.)

K10 NAME Name of fissionable isotope for which a fission neutron spectrum is to be read in as input. The fissionable isotopes

in KAPER include αTH320α, αU2330α, αU2340α, αU2350α, αU2360α, αU2380α, αPU390α, αPU400α, αPU410α and αPU420α. See Section VII for clarifications.

K11 (CHI(K),K=1,NOG) Fission neutron spectrum, by energy group, for isotope NAME.

S2 End of card input for phase 99999.

K12 NI Number of isotopes for which a new temperature, for the Maxwellian shape of the fission neutron spectrum, is to be read as input.

NE >0; Read in new energy group boundaries for the group structure of the cross section set used.

S3 If NE>0 input card K13, otherwise go to card K14.

K13 N Number of new energy limit values to be read in.

(E(K),K=1,N) Upper energy limit of the $K^{\underline{th}}$ energy group (MeV).

S4 If NI>0 input card K14, otherwise end of card input for phase 99999.

(Card K14 is repeated NI times.)

K14	NAME	Name of fissionable isotope for which a new Maxwellian temperature is to be read in. The name convention is the same as on card K10.
	TEMP	Maxwellian temperature (MeV) for isotope NAME.

S5 End of card input for phase 99999.

3) Phase 99998, flux, adjoint and reaction rate phase. In this portion of the program the flux and adjoint distributions in the heterogeneous cell are calculated, as well as heterogeneous reaction rates if they were specified during the cross section preparation in phase 99999. If the cross section prepared in phase 99999 are for a homogeneous mixture the program will automatically select the correct computational path. In either case the card input in this phase remains the same.

K1	α99998α	Constant
K2	NFPH	Number of the following phase
	NHØM	>0 for quasi-homogeneous calculations in which the optical thickness of the cell is less than or equal to 10^{-4}, otherwise 0.

NXST — External unit number which contains cross sections for the normal cell. When fluxes from this calculation are to be used in the reactivity worth phase, NXST must be a positive number. In this case the cross sections are saved and the fluxes are written on NXST for transfer to phase 99997. For all other calculations enter NXST as a negative number. When NXST is negative the adjoint distribution in the cell is not calculated.

NPERT — External unit number which contains cross sections for the perturbed cell. This is an option which can be used to calculate flux and reaction rate distributions in a cell inserted between the normal repeating cells of the assembly but which is different, in some manner, than the normal cell. When the perturbed cell option is not used NPERT must be zero.

IB — 0 No Bucklings are to be used, therefore leakage is set equal to zero.

1 Universal Buckling to be used

>1 Group dependent Bucklings to be used (In the case IB≥1 input card K4 or K5)

KBSQ — >0 Iteration on Buckling (B^2) to a desired k_{eff} as specified on card K6, otherwise 0.

NGC — 1 If the perturbed cell, as defined on unit NPERT, is to be extended by a normal cell on each side (from unit NXST) before

		calculation of the flux distribution in the perturbed cell. This option can be used to investigate the influence of the perturbed cell boundary selection without redefining the cell in phase 99999. 0 For all other cases.
	IAN	1 Anisotropic leakage considered and directional diffusion coefficients calculated. If this option is selected and Bucklings are input be sure to see comment S1. The diffusion coefficient is calculated parallel and perpendicular to the plate structure. 0 Otherwise
	IHCS	>0 The cross sections for the heterogeneous cell are homogenized for use in a succeeding calculation, e.g. in a one-dimensional diffusion theory program. (Input card K7 and K8) 0 Otherwise
K3	IMIN	Minimum number of outer iterations for convergence on the eigenvalue (IMIN≥3)
	IMAX	Maximum number of outer iterations
	EPSCON	Convergence criterion for the fluxes
	EPS	Convergence criterion for the eigenvalue (k_{eff})

S1 If NB=0 go to S3, otherwise go to K4 if IB=1 or to K5 if IB>1. If IAN=1 cards K4 and K5 consist of two cards each. The first and second cards are, respectively, the Buckling (B^2) parallel and perpendicular to the plate structure. Normally, as in the SNEAK assembly, they are the radial and axial B^2 respectively.

K4	BSQ	Universal Buckling

S2 Go to S3

K5	(BSQ(K),K=1,NOG)	Group dependent Buckling, where NOG is the number of energy groups.

S3 If KBSQ=0 go to S4, otherwise input card K6.

K6	MAXB	Maximum number of iterations on the Buckling to the specified k_{eff}.
	AKE	Desired k_{eff}
	EBK	Convergence criterion for k_{eff}
	FAB	Factor used to multiply the initial Bucklings for a second guess of the Bucklings (recommended FAB=1.1 to 1.2).
	NBQ	Group number (arbitrary) in which the Buckling is positive.

S4 If IHCS=0 end of card input for phase 99998, otherwise input card K7.

K7 NPT — External unit number on which the homogenized cross sections are to be written. NPT may be the same unit number as NXST if the data presently on it is no longer needed at this point.

IRR — Number of isotopes for which homogenized reaction rate cross sections are to be calculated. The first IRR isotopes of the NOR isotopes specified on card K9 of phase 99999 will be treated. (IRR$\leq$NØR)

IM — Number of homogenized cross section sets produced. (IM$\leq$3). It is possible to produce up to three sets in which all the cross sections are identical except for the diffusion coefficient as determined by MD(I).

(MN(I), — Number assigned to this set of cross sections.

MD(I), — Diffusion coefficient for this set

0; $\hat{D} = \frac{2}{3} D_{||} + \frac{1}{3} D_{\perp}$

1; $\hat{D} = D_{\perp}$ (perpendicular)

2; $\hat{D} = D_{||}$ (parallel)

I=1,IM) — The diffusion coefficient is not written on the unit NPT, but rather the transport cross section is calculated from the diffusion coefficient specified and is written on NPT ($\Sigma_{tr} = \frac{1}{3\hat{D}}$).

S5 If IRR=0 end of card input for phase 99998, otherwise input K8.

K8 (NARR(I),I=1,IRR) Material combination name (8-byte word) assigned to the homogenized reaction rate cross sections.

The homogenized cross sections, as specified on cards K7 and K8, are written on unit NPT in a form that can be read directly by phase α00451α of the Karlsruhe NUSYS program system. The variable MN(I) is the composition number of the cross sections in the SIGMA block of NUSYS which will be replaced by the KAPER cross sections. For clarity the form of the cross sections on unit NPT is given. For each cross section type one record is written as shown below. The form of the records are:

Record type R_1 (format free)

NA1 = SIGMA (constant 8-byte word)

NA2 = cross section type name (8-byte word) which include the following:

- SCAPT = total absorption, capture plus fission
- NUSF = nu sigma fission
- STR = transport cross section
- SREM = total group removal
- SFISS = fission (always set equal to zero)
- CHI = fission neutron spectrum
- SMTOT = scattering matrix

IS = column index for the scattering matrix, for other cross section types IS=0.

NA3 = MAGRO (constant 8-byte word)

MN(I) = composition number assigned to this cross section set (see card K7)

NOG = number of energy groups

((IG, = group index

SX(IG)),IG=1,NOG) = respective cross section value

Record type R_2 (format free)

NA1 = SRATE (constant 8-byte word)

NA2 = reaction rate cross section type name (8-byte word) which include the following:

- SCAPT = capture cross section
- SFISS = fission cross section

IS = 0 constant

NARR(I) = constant 8-byte word (see card K8)

MN(I) = composition number assigned to this cross section set (see card K7)

NOG = number of energy groups

((IG, = group index

SX(IG)),IG=1,NOG) = respective cross section value

The order in which the records are written on unit NPT is the following:

1) 1 record containing two words

IX = (6+NOG)*IM+IRR*2*IM (total number of records on unit NPT excluding the first)

NOG = number of energy groups

2) IM records of type R_1 for NA2 = CHI

3) 5 records of type R_1 for NA2 = SCAPT
NA2 = NUSF
NA2 = STR
NA2 = SREM
NA2 = SFISS
respectively.

4) NOG records of type R_1 for NA2 = SMTOT with the index IS running from 1 to NOG.

Note: 3) and 4) are repeated then (IM-1) times, once for each composition number (MN(I)) selected. The cross sections are the same except for the transport cross section which is defined by MD(I) of card K7.

5) 2 records of the type R_2 for NA2 = SCAPT and NA2 = SFISS respectively.

Note: 5) is repeated for each of the IRR isotopes for which reaction rate cross sections are produced.

4) Phase 99997, Reactivity Worth Phase. In this phase heterogeneous reactivity worths are calculated. If homogeneous cross sections were prepared in phase 99999 the program will perform a homogeneous first-order perturbation calculation automatically. In this case a number of the variables as input on the following cards have no meaning as is noted.

K1	α99997α	Constant
K2	NFPH	Number of following phase
	NFLUX	External unit number containing cross sections and fluxes for normal cell. Normally NFLUX=NXST on card K2 of phase 99998.
	NPERT	External unit number containing cross sections and fluxes for the perturbed cell. Normally NPERT=NPERT on card K2 of phase 99998. When option is not used NPERT=0. In this case the program substitutes a normal cell for the perturbed cell and, therefore, all remarks pertaining to the perturbed cell in the following input data apply to the substituted normal cell (does not apply in homogeneous case).
	NXECT	External unit number containing cross sections for the various samples to be calculated.

NTAPE

Reserve external unit for collision probabilities. The space needed on this unit is SPACE (bytes) = 4*NOG*IOX*IOX where

NOG = number of energy groups

IOX = 2*NCELL*NY+NW

NCELL = input data

NY = number of regions into which the normal cell is divided

NW = number of regions into which the perturbed cell is divided.

NTAPE1

Reserve external unit for collision probabilities. The space needed on this unit is the same as computed for NTAPE.

NSAM

Number of samples to be calculated. This is the number of cross section sets on unit NXECT.

NFP

Maximum number of fissionable isotopes in any one cross section set on unit NXECT.

NCELL

Number of normal cells (≥ 1) to be placed on either side of the perturbed cell for the calculation of the reactivity effects. It is for these cells that the range of the terms δP_{ij} are defined. NCELL should be large enough so that the probability a neutron from the perturbed cell suffers a collision before reaching the outer boundary of the last normal cell is at least 0.98. If the parameter is given as NCELL<0 the program will select an appropriate value for it.

K3	IH	1; Flux and adjoint distributions are to be superimposed on a cosine group-dependent curve. This curve is defined by the bucklings given on card K4 or K5 of phase 99998 as f(x)=cos(Bx) where the center point, x=0, is located at the center of the cell containing the sample. 0; Option not used
	IH1	1; Perturbed flux calculated and used in perturbation calculation. 0; Unperturbed flux (as calculated in phase 99998) used in perturbation calculation.
	MORE	1; Cross sections and/or region dimensions are to be changed for the perturbed cell as they are transfered from phase 99998. 0; Option not used -1; A void is specified in one or more regions of the perturbed cell with card K5.
	NUNPER	When MORE=1, external unit number with new cross sections and/or region dimensions for the perturbed cell as prepared from phase 99999. For MORE≠1, the parameter NUNPER is meaningless.
K4	ENORM	This variable is used to normalize the reactivity values to the results of a multi-dimensional calculation. Normally ENORM is equal to the following

$$\text{ENORM} = \frac{S_f(o)\ S^+(o)}{\int d^3r\ S_f(\bar{r})\ S^+(\bar{r})}$$

where $S_f(\bar{r})$ and $S^+(\bar{r})$ are the fission and adjoint sources, respectively, and the integration is over the reactor core and reflector.

S1 If MORE≠-1 go to card K6, otherwise input card K5.

K5 (VOID(I),I=1,NW) VOID(I)=0.0 for the $I^{\underline{th}}$ region in which a void is desired in the unperturbed state, otherwise set VOID(I)=1.0, where I=1,NW are the region indices of the perturbed cell. It is possible to use VOID(I) to adjust the density of the $I^{\underline{th}}$ region by simply putting VOID(I) equal to an appropriate value, e.g., to reduce the density in the $I^{\underline{th}}$ region by a factor of 2, VOID(I)=0.5.

Card K6 is repeated NSAM times with a descriptive title for each sample in the order in which they are calculated.

K6 NT Number of four character words in the description title ($\leq$15)

(TITLE(I),I=1,NT) The title must be placed between apostraples (') and can consist of any character except apostraples. An example of this is shown

e.g. (7 'SNEAK-900A_WORTH_FOR_U-238')

End of card input for phase 99997.

III. Computer Core Space Requirements

The KAPER program requires 130K bytes of core storage for the overlay structure suggested in this guide, plus N_1, N_2, or N_3 whichever is the largest. The values of the N's are defined by the following equations for each phase of the program.

1) Phase 99999; cross section phase

$$N_1 = 4*\left[NIS*NOG*(39+NOG)+10*NR*NR+78*NR+(20+NR)*NOG+6\right]$$

where NIS = number of isotopes
NOG = number of energy groups
NR = number of regions

2) Phase 99998; flux, adjoint, and reaction rate phase

$$N_2 = 4*\left[NOG*NR*(NOG+NR+13+NFI+2*NRS)+NOG*(12+NFI)+8+NR*(5+NFI+NRS)+IAR*IAR\right]$$

where NOG = number of energy groups

NRS = number of isotopes for reaction rate calculations; NRS=NOR on card K3 in phase 99999 if NOR>0, or NRS=1 if NOR=0.

NR = number of regions (NR=MAX(NY,NW) where NY is the number of regions in the normal cell and NW is the number of regions in the perturbed cell. If NGC=1 then NR=2*NY+NW, see card K2 of phase 99998).

IAR = NY if IAN=1, otherwise IAR=1 (see card K2 of phase 99998).

NFI = number of fissionable isotopes in the cells.

3) Phase 99997; reactivity worth phase

$$N_3 = 4*\lceil NOG*NR*(4+NF)+NOG*NW*(4+NFP) +NOG*NOG*(NW+NR)+IXO*(2*IXO+NOG+2) +NR*2+NOG*(14+NF+2*NFP)+NR*MAF +NOG*I1*I1+1\rceil$$

where NY = number of regions in the normal cell

NW = number of regions in the perturbed cell, if the perturbed cell option in the phase 99998 is not used then NW=NY

NR = NY+NW

IXO = 2*NCELL*NY+NW where NCELL is defined on card K2 of phase 99997

NOG = number of energy groups

NF = number of fissionable isotopes in the normal cell

NFP = maximum number of different fissionable isotopes
in any one set of data for sample reactivity worths
(see card K2 of phase 99997)

MAF = MAX(NF,NFP)

I1 = MAX(NY,NW)

In the above equations for the N's the formulation

$$X = MAX(Y_1, Y_2, Y_3, \ldots)$$

means that the maximum value of the Y variables is assigned to X. The N's are computed in bytes. The PARM.G in the EXEC card (see the section IV. on control cards) is set equal to, or greater than, the largest of N_1, N_2, or N_3. In other words

$$PARM.G = MAX(N_1, N_2, N_3).$$

The REGION size is then PARM.G plus 130K for the program.

IV. Control Cards and Deck Structure

The following is a list of the necessary control cards needed for a normal calculation. In these cards a blank is denoted with _. In this example the compiled program is found on the tape DV0377.

```
//"Job Card"
/*SETUP_DEVICE=TAPE9,ID=(DVO377,NØRING,SAVE,SL)
//_EXEC_FHLG,PARM.L='ØVLY',PARM.G=XXXXXX,TIME.G=XX
//L.SYSUT1_DD_SPACE=(3303,700)
//L.SYSLMØD_DD_SPACE=(3303,700,,1))
//L.KAPER_DD_DSN=KAPER,UNIT=TAPE9,VØL=SER=DVO377,
//_DISP=(ØLD,PASS)
//L.SYSIN_DD_*
_ENTRY_MAIN
_INCLUDE_KAPER
_ØVERLAY_A
_INSERT_DUMMY3,PPM760,PPM761,SPEK,GRREAP,INPØØ
_INSERT_INDX,PMC,BRB,CH,M10760,NSPEK
_ØVERLAY_A
_INSERT_DUMMY2
_ØVERLAY_B
_INSERT_HØMØCA
_ØVERLAY_B
_INSERT_HET
_ØVERLAY_B
_INSERT_QUERP
_ØVERLAY_B
_INSERT_HETERØ,TABLE,ASLAB,BENØIS,SLAB,SLABP,E5,EZ5
_INSERT_PE5,E4,YZ5
_ØVERLAY_A
_INSERT_DUMMY1
```

```
_ØVERLAY_B
_INSERT_CELLØ
_ØVERLAY_B
_INSERT_DEMØ,PEFLUX,SLOO1,SLOO2,CPERT,CØLL,PERT
_ØVERLAY_B
_INSERT_HØMPET
//G.FTO8FOO1_DD_UNIT=SYSDA,SPACE=(TRK,(9))
//G.FTO4FOO1_DD_DSN=GROUCO,VOL=SER=NUSICE,UNIT=3330,
//_DISP=SHR
   .
   .
   .
   plus needed units for data transfer
   .
   .
   .
//G.SYSIN_DD_*
   .
   .
   .
   Input cards
   .
   .
   .
/*
```

The declaration of unit 8 is always necessary since the input cards are transfer to it for reading by the program without format control. The unit number 4 must always be declared as it is the cross section library.

V. Program Structure and Operation

The KAPER consists of the main program and many subprograms as shown on the overlay map, Fig. 1. In this section a brief description of the function of the various subprograms is given.

MAIN

This program controls the logical sequence of the code. Here the maximum amount of core storage is allocated for the problem based on the information supplied by the user. Calling of the three segments (phases 99999, 99998, and 99997) is performed as specified by the card input.

PARM (called from MAIN)

PARM is an assembler program which reads the contents of the PARM.G field on the EXEC card for use within a FORTRAN program.

CONVY (called from MAIN)

The subprogram performs a conversion from machine internal fixed or floating point to alphanumerical, or the reserve.

ALLOCX (called from MAIN)

Dynamic assignment of main core storage at execution time.

FREEX (called from MAIN)

Release of dynamically assigned main core storage.

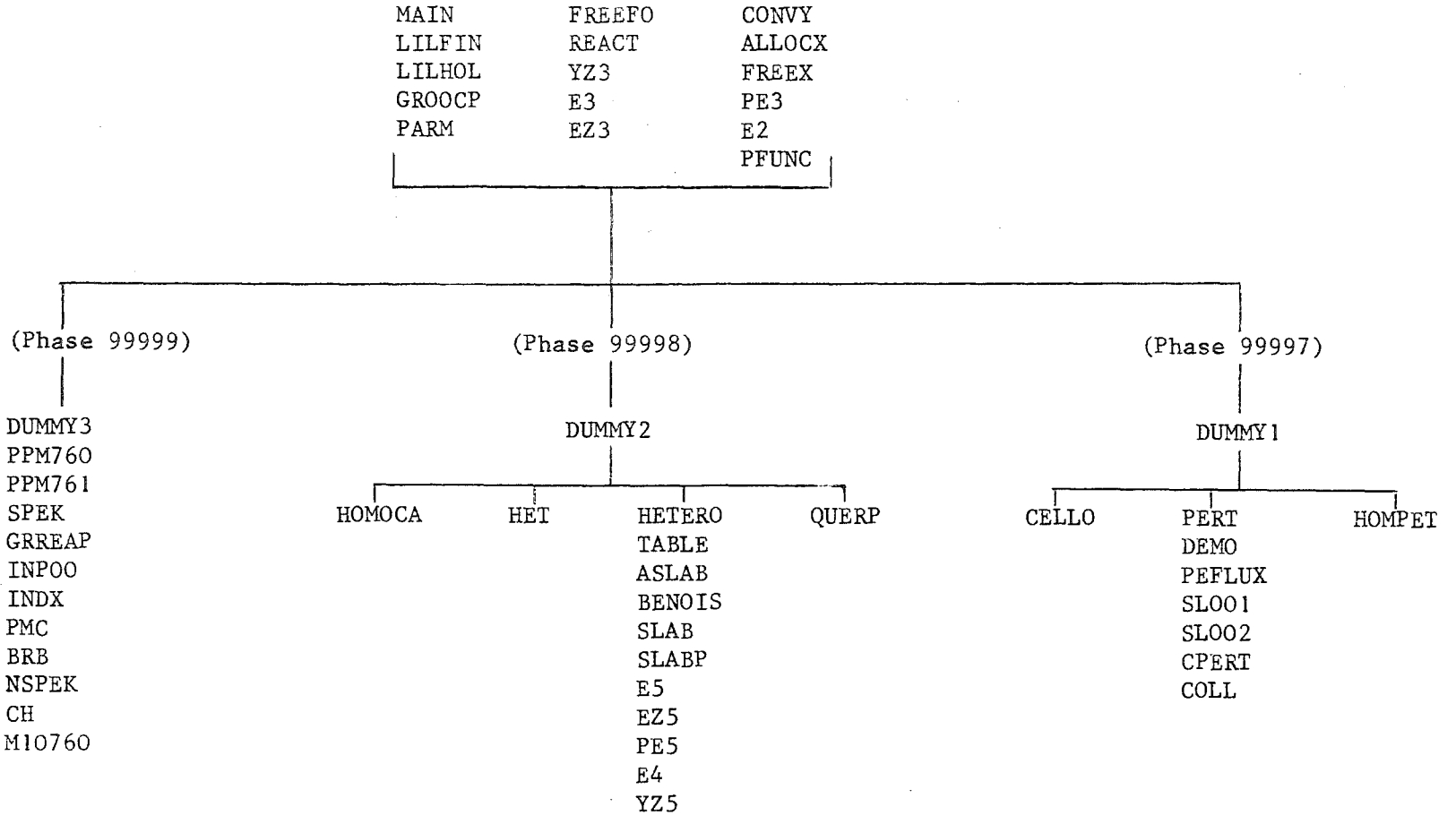

Fig. 1 Recommended Overlay Structure for KAPER

FREEFO (called from MAIN)

This subprogram reads all card input without control of format and transfers the data to a temporary unit assigned the number 8. All subsequent read statements for card input refer to this temporary unit.

LILFIN (called by DUMMY3, DUMMY1, DUMMY2)

LILFIN determines the next segment of the overlay program required to continue the calculation.

LILHOL (called from GRREAP)

Used to place a literal constant in a particular variable address.

GROOCP (called from GRREAP)

Reading of group microscopic cross section data from the cross section library.

REACT (called from HETERO and HOMOCA)

In this subroutine space-dependent reaction rates in the cell are calculated and printed. In addition the integral flux and cell averaged reaction rates are calculated.

YZ3 (called from SLAB, ASLAB, and SLOO1)

A routine for the calculation of the difference of the infinite sums of exponential integrals of order 3.

E3 (called from SLAB, ASLAB, PE3, SLABP, DEMO, SLOO1, SLOO2, COLL)

Calculation of exponential integrals of order 3 ($E_3(x)$)

EZ3 (called from YZ3)

Infinite summation of exponential integrals of order 3.

PE3 (called from EZ3)

Evaluation of exponential integral of order 3 for small arguments.

E2 (called from EZ3, YZ3, EZ5)

Calculation of exponential integral of order 2 ($E_2(x)$).

PFUNC (called from YZ3)

The probability of escape without a collision from a slab.

DUMMY3 (called from MAIN)

This subprogram provides the control for this segment of the overlay program. The input cards for this phase of the calculation are sampled and the core storage needed for the problem is determined. The relative addresses of the variables are calculated and passed to the subprograms of this segment.

PPM760 (called from DUMMY3)

Reading of all input data on cards for problem in phase 99999 is performed in this subprogram. Some checks are performed on input data.

GRREAP (called from PPM760)

Assignment of locations for cross section data from the cross section library is done as well as the calculation of certain cross section types not given directly in the library.

PPM761 (called from DUMMY3)

This large subroutine calculations the heterogeneous resonance self-shielded cross sections and stores them on an external unit for use in subsequent segments (DUMMY1 or DUMMY2).

SPEK (called from PPM761)

Determination of location in COMMON/CH/ of fission neutron spectra for the individual fissionable isotopes in a calculation.

NSPEK (called from PPM761)

NSPEK calculates fission neutron spectra from a Maxwellian distribution.

INPOO (called from PPM761)

A routine for the interpolation of resonance self-shielding factors.

INDX (called from PPM761)

This routine is for indexing of reaction coefficients used in the calculation of effective cross sections.

BRB (called from PPM761)

This is a routine for the determination of the coefficients in the fitting of a series of partial factions to the collision probabilities.

PMC (called from PPM761)

In PMC collision probabilities, for use in the determination of effective cross sections, are calculated.

CH

This is a BLOCK DATA routine used to initialize a common block having fission neutron spectra, with corresponding Maxwellian temperatures, and the energy group limits of the 26-group structure of the Karlsruhe cross section set.

M10760

Common block used in the segment controlled by the subprogram DUMMY3.

DUMMY2 (called from MAIN)

This subprogram provides the control for this segment of the overlay program. The input cards for this phase of the calculation are sampled and the core storage needed for the problem is determined. The relative addresses of the variables are calculated and passed to the subprograms of this segment.

HET (called from DUMMY2)

All input data, cards, and cross sections from PPM761, are read in by HET. Printing of initial variables for the problem is performed.

HOMOCA (called from DUMMY2)

This routine performs a zero-dimensional homogeneous calculation of flux and adjoint.

QUERP (called from DUMMY2)

Homogenized cell cross sections are calculated and stored on an external unit for later use in multi-dimensional computer codes. The homogenized cross sections include macroscopic cell cross sections, average fission neutron spectrum for the cell, and reaction rate cross sections.

HETERO (called from DUMMY2)

The flux and adjoint in the heterogeneous cell are calculated in HETERO. A neutron balance in the cell is also calculated.

For the case that reactivity worths are desired the cell normalization integral (perturbation denominator) is calculated.

TABLE (called from HETERO)

A table of exponential integrals of order 3, 4, and 5 are calculated from two polynomials over a discrete mesh spacing, and are stored in a common block for use by the collision probability routines. In addition the weights and modes of the Gaussian Quadrature approximation to the infinite summation of the exponential integrals are initialized.

ASLAB (called from HETERO)

The collision probabilities for a cell in an infinite repeating lattice are calculated.

BENOIS (called from HETERO)

The components of the diffusion coefficient (parallel and perpendicular to the plate structure) are calculated using the first term of the Benoist formulation (see Eq. (2.12) in Section VI.).

SLAB (called from HETERO)

The collision probabilities of a perturbed cell located in an infinitely repeating lattice of normal core cells are calculated.

SLABP (called from HETERO)

The collision probabilities within a single unit cell are calculated for neutrons originating only within the cell.

E5 (called from PE5 and BENOIS)

Calculation of exponential integral of order 5 ($E_5(x)$).

EZ5 (called from YZ5)

Infinite summation of exponential integrals of order 5.

PE5 (called from EZ5)

Evaluation of exponential integral of order 5 for small arguments.

E4 (called from EZ5)

Calculation of exponential integral of order 4 ($E_4(x)$).

YZ5 (called from BENOIS)

A routine for the calculation of the difference of the infinite sums of exponential integrals of order 5.

DUMMY1 (called from MAIN)

This subprogram provides the control for this segment of the overlay program. The input cards for this phase of the calcu-

lation are sampled and the core storage needed for the problem is determined. The relative addresses of the variables are calculated and passed to the subprogram of this segment.

CELLO (called from DUMMY1)

This subroutine calculates the space requirements for the collision probabilities.

PERT (called from DUMMY1)

The input cards are read for the calculations as well as the data (cross sections and fluxes) from the phases 99999, and 99998. Printing of initial variables is performed.

DEMO (called from PERT)

The normalization integral (perturbation denominator) is calculated for the cell under the assumption that the flux and adjoint have a curvature (cosine) away from the cell as given by the Buckling.

PEFLUX (called from PERT)

The perturbed flux in the cell containing the sample is calculated. The environment of the cell containing the sample is taken as an infinite repetition of normal core cells.

SLOO1 (called from PEFLUX)

Collision probabilities of the cell, containing the sample, located in an infinitely repeating lattice of normal core cells are calculated.

SLOO2 (called from PEFLUX)

The collision probabilities within the sample cell are calculated for neutrons originating only within the cell.

COLL (called from PERT)

The collision probabilities for the two cases, sample in and sample out, are calculated for use in the perturbation theory calculation. They are written on an external unit for use in subroutine CPERT.

CPERT (called from PERT)

The reactivity worth of a sample is calculated with integral transport perturbation theory.

HOMPET (called from DUMMY1)

This routine is a homogeneous version of the CPERT routine for the calculations of reactivity worths. A homogeneous formulation of perturbation theory is utilized.

VI. Computational Methods Utilized in KAPER

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KAPER - A COMPUTER PROGRAM FOR THE ANALYSIS OF EXPERIMENTS PERFORMED IN HETEROGENEOUS CRITICAL FACILITIES

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Abstract

The essential features of the methods employed to calculate effective multigroup self-shielded cross sections, flux and reaction rate distributions, and reactivity worths in a heterogeneous cell are presented. The methods are based on a heterogeneous formulation of the self-shielding factor ("f-factor") concept in the integral transport theory equation. Representative numerical results are included and compared to experiments.

1. Introduction

The KAPER program /1/ is a multigroup lattice code developed to analyze experiments performed in plate-type heterogeneous critical facilities. These experiments include those in which the flux fine structure in the lattice must be taken into account, as for example in reaction rate and small-sample reactivity worth measurements. The program may also be used to provide homogenized heterogeneous resonance self-shielded cross sections for multidimensional diffusion or transport codes. This paper provides a discussion of the methods employed in the program. Included also is a comparison of results from KAPER with results of experiments and other computer codes. Some typical results of experiments analyzed with KAPER are given.

The program is a dynamically dimensioned code in an overlay structure. The three main segments consist of a procedure for the calculation of resonance self-shielded cross sections in the multiregion cell, a procedure for the calculation of the cell fluxes (real and adjoint) including reaction rates, and a procedure for the calculation of small-sample reactivity worths.

The fundamental basis of the program is integral transport theory in the collision probability formulation. The multigroup resonance self-shielded cross sections for the multiregion cell are defined by a procedure utilizing the "f-factor" concept. The concept of the composition-dependent self-shielding factor ("f-factor") for homogeneous media was first introduced by Abagjan et al. /2/ and recently tested against a more exact model by Kidman et al. /3/. A consistent formulation for the heterogeneous medium was developed through

the integration of the space and energy dependent integral transport equation and represents an improvement in a method originally developed by Wintzer /4/.

The program has a particular feature which allows one to calculate the flux distributions (real and adjoint) and reaction rates in a cell differing from the normal unit cell of the core. This feature has great utility for analyzing experiments that disturb the properties of the cell in the measurement procedure. In this problem the flux is found by solving the integral transport equation as a fixed source equation in which the normal unit cell serves as an external source.

Reactivity worths are calculated with an exact perturbation formulation of the integral transport equation. By exact is meant that the perturbed flux and unperturbed adjoint are used in the formulation.

2. Calculation of Heterogeneous Cross Sections and Fluxes

The equations used for cell calculations in the KAPER program are derived from the energy dependent integral Boltzmann equation, which is in the case of isotropic scattering,

$$\Sigma_t(E,r)\Phi(E,r) = \int d^3r'\ S(E,r')\ P(r' \to r,E) \tag{2.1}$$

where Φ is the flux, S is the neutron source density, Σ_t is the total cross section, and P is the first-flight collision probability. The source density is composed of the fission source and the slowing down source in the following manner

$$S(E,r) = \int dE' \left[\Sigma_s(E' \to E,r)+\lambda\chi(E)\nu\Sigma_f(E',r)\right] \Phi(E',r) \tag{2.2}$$

where λ is the eigenvalue. The remaining notation is standard.

To obtain the multigroup equations for a fast reactor system, where resonance effects are important, one usually postulates the narrow resonance approximation and observes that the source density S shows no resonance structure within this approximation. Then, the straightforward procedure is to eliminate the flux Φ between Eqs. (2.1) and (2.2) and to write the multigroup equations with the source density S as a variable. If the unit cell is subdivided into N regions with index n, the resulting equations are

$$V_n S_n^g = \sum_m \sum_k V_m S_m^k \left[\left\langle \frac{\Sigma_{s_n}^{k\to g}}{\Sigma_{t_n}}(E)\ P_{mn}(E) \right\rangle_k + \lambda\chi^g \left\langle \frac{\nu\Sigma_{f_n}}{\Sigma_{t_n}}(E)\ P_{mn}(E) \right\rangle_k \right] \tag{2.3}$$

where V_n is the volume of the $n^{\underline{th}}$ region and g is the energy group index. The brackets $\langle\ \rangle$ indicate averages over energy. The problem of the weighting spectrum within the energy group will not be discussed here.

For reasons which will be explained later an alternative procedure to that above is used in KAPER; it consists of eliminating the source densities S between Eqs. (2.1) and (2.2). One then obtains the following equations for the neutron flux

$$V_n \Sigma_{t_n}^g \phi_n^g = \sum_m P_{mn}^g \sum_k \left[\Sigma_{s_m}^{k\to g}+\lambda\chi^g\nu\Sigma_{f_m}^k\right] V_m \phi_m^k \tag{2.4}$$

where $P^g_{mn} = \langle P_{mn}(E) \rangle_g$
and the effective cross sections $\Sigma^g_{x_n}$ are defined by

$$\Sigma^g_{x_n} = \frac{\sum_m \left\langle \frac{\Sigma_{x_n}}{\Sigma_{t_n}}(E)\ P_{mn}(E) \right\rangle_g V_m S^g_m}{\sum_m \left\langle \frac{1}{\Sigma_{t_n}}(E)\ P_{mn}(E) \right\rangle_g V_m S^g_m} \tag{2.5}$$

It must be emphasized that the two systems of equations, Eqs. (2.3) and (2.4), are completely equivalent within the narrow resonance approximation. Both Eq. (2.3) and Eq. (2.4) can be readily solved if the coefficients are available. However for a typical cell of a fast critical assembly, where resonance absorbers may be present with different concentrations in several regions of the cell, the calculation of these coefficients can be a difficult problem. In this type of problem the usual equivalence theorem of resonance absorption is no longer valid and one has to search for more elaborate methods to calculate the self-shielding in the different regions.

For the calculation of the coefficients in the KAPER program we have modified a method which was originally proposed by D. Wintzer /4/, and which is used in the Karlsruhe code ZERA.

In Wintzer's method, the coefficients of Eq. (2.3), here written as A_{xmn} for a particular reaction rate of type x, are constructed from the contributions of the individual isotopes. Thus, one has

$$A_{xmn} = \left\langle \frac{\Sigma_{xn}}{\Sigma_{tn}}(E)\ P_{mn}(E) \right\rangle = \sum_\nu A_{x\nu mn}, \tag{2.6}$$

where the summation is over isotopes. Each isotopic $A_{x\nu mn}$ can be written as

$$A_{x\nu mn} = \left\langle \frac{\sigma_{x\nu}(E)}{\sigma_{on} + \sigma_{t\nu}(E)}\ P_{mn}\ (\sigma_{t\nu}(E), \sigma_o) \right\rangle \tag{2.7}$$

where $\sigma_{t\nu}$ is the total cross section of the isotope ν, and σ_{on} is the "background" cross section, per atom of isotope ν, due to the other isotopes present in region n. The background cross section σ_{on} is assumed constant in energy. Note that the collision probability P_{mn} depends on the background cross sections of all other isotopes present between the regions m and n; this dependence is indicated by σ_o.

The main point in Wintzer's method is that the functions involving the collision probabilities are fitted to a sum of partial fractions

$$\frac{1}{\sigma_{on} + \sigma_{t\nu}(E)}\ P_{mn}(\sigma_{t\nu}, \sigma_o) \approx \sum_{i=1}^{I} \frac{a_i}{b_i + \sigma_{t\nu}(E)} \tag{2.8}$$

With this approximation, the averaging over resonances can be easily carried out. The resulting expressions are related to the self-shielding factors by the equation

$$\left\langle \frac{\sigma_{x\nu}}{b_i + \sigma_{t\nu}} \right\rangle = \frac{\langle \sigma_x \rangle_\nu \, f_x(b_i)}{b_i + \langle \sigma_t \rangle_\nu \, f_t(b_i)}$$

where $f_x(b_i)$ is the tabulated self-shielding factor for a background cross section having the value b_i and $\langle \sigma \rangle$ is the infinitely dilute cross section (i.e. no resonance self-shielding).

This method of Wintzer's works well for lattices with weak heterogeneity, but it fails if the heterogeneity is large, that is, if the optical thickness of at least one region is large. The reason is that the coefficients $A_{x\nu mn}$ depend fairly strongly on the background cross section, which is not well defined. Presently the unshielded total cross sections are generally used as background cross sections.

Therefore, an improvement in Wintzer's method was proposed, and is used in the KAPER program. The coefficients $A_{x\nu mn}$ are calculated as described above. Then, the effective self-shielded cross sections for each reaction, region, and isotope are obtained from the equation

$$\tilde{\sigma}_{x\nu n} = \frac{\sum_m \left\langle \frac{\sigma_{x\nu}}{\sigma_{on} + \sigma_{t\nu}} P_{mn}(\sigma_{t\nu}, \sigma_o) \right\rangle V_m S_m}{\sum_m \left\langle \frac{1}{\sigma_{on} + \sigma_{t\nu}} P_{mn}(\sigma_{t\nu}, \sigma_o) \right\rangle V_m S_m} \qquad (2.9)$$

These cross sections are used in Eq. (2.4). The collision probabilities P_{mn} occurring in Eq. (2.4) are calculated with the self-shielded total cross sections.

The approximation of Eq. (2.9) is good since the effective cross sections depend only very weakly on the background cross sections. This was observed for a similar homogeneous case in /5/ and is demonstrated for the heterogeneous cases in the results of Section 5 of this paper. Thus it is possible to say that the self-shielded cross sections are fairly well defined by Eq. (2.9). It is for this reason that Eq. (2.4) is used in KAPER rather than Eq. (2.3) with its coefficients which are sensitive to the background cross sections.

The use of the self-shielded total cross section, Eq. (2.9), to calculate the collision probabilities is an approximation which we could not derive from mathematical principles; however we feel that the approximation is adequate for the purposes of practical calculations.

It should be noted that the procedure outlined above, as used in KAPER, is the first step of a rapidly converging iterative method which consists of using the self-shielded total cross sections, Eq. (2.9), to obtain the background cross sections in Eqs. (2.7) and (2.8), and then repeating the entire procedure. In this manner one could derive a consistent set of self-shielded cross sections; the KAPER cross sections are very close approximations to this consistent set.

The source densities S_m, which appear in Eq. (2.9), are first approximated in KAPER by the fully self-shielded total cross sections

$$S_m = \sum_\nu N_{\nu_m} \sigma_{t\nu} \quad (\sigma_o = o) \qquad (2.10)$$

An iteration on the source densities can be carried out if required. However, in most cases, the first approximation, Eq. (2.10), is sufficiently good.

The heterogeneous flux distribution within a unit cell is calculated by solving Eq. (2.4) with the cross sections defined by Eq. (2.9). The equation is solved by the power iteration method. Convergence is assumed when the following condition is fulfilled in an outer iteration

$$\left| 1 - \frac{(\alpha^{(i-1)})^2}{\alpha^{(i)}\ \alpha^{(i-2)}} \right| \leq \varepsilon$$

where $\alpha^{(i)}$ is the total cell fission source for the i^{th} iteration. The equation adjoint to Eq. (2.4)

$$\Sigma_{t_n}^{g} \phi_n^{+g} = \sum_m \sum_k P_{nm}^{k} \left[\Sigma_{s_n}^{g \to k} + \lambda \chi^k \nu \Sigma_{f_n}^{g} \right] \phi_m^{+k} \qquad (2.11)$$

is solved in an analogous manner. Because the collision probabilities in all the equations are calculated exactly there is no assumption made about the flux, or neutron current, at the boundary of the cell. The procedures used to evaluate the collision probabilities are based on the methods developed by A.P. Olson /6/ for the RABID code.

In KAPER, Eqs. (2.4) and (2.11) are used in a slightly more refined form for the fission source. The fission spectrum, χ^g, used in multigroup equations should be a properly weighted spectrum derived from the contributions of the various fissionable isotopes present in the unit cell. Generally the correct spectrum is not known a priori and must, therefore, be approximated. To circumvent this problem the KAPER program uses a fission spectrum for each particular fissionable isotope present in the unit cell and calculates the fission source in energy group g and region m as

$$\sum_j \chi_j^g \sum_k \nu \Sigma_{f_{j_m}}^{k} V_m \Phi_m^k$$

where j is the fissionable isotope index. This representation of the fission source is particularly important in the calculation of reactivity worths (Section 4). For example, the use of a universal fission spectrum for the calculation of uranium sample worths in an assembly, whose predominant fission source is from the plutonium isotopes, can result in a 2% error even if the universal fission spectrum is correctly weighted. The above representation of the fission source is used throughout the KAPER program. For simplicity, however, the fission sources in this paper are written with a universal fission spectrum.

To account for leakage, the collision probabilities are scaled in the following manner:

$$P_{mn} \to \frac{\overline{\Sigma}_t}{\overline{\Sigma}_t + \overline{D}B^2} P_{mn}$$

where $\overline{\Sigma}_t$ and $\overline{D}$ are defined as cell flux-averaged quantities. Since the fluxes needed to calculate $\overline{\Sigma}_t$ and $\overline{D}$ are not known a priori the calculation of the

scaling factor is included in the outer iteration procedure in the solution of the flux equation.

In some experiments performed in critical assemblies the anisotropic effect of diffusion, resulting from the orientation of the platelets composing the assembly, plays an important role. To account for this effect the $\overline{DB}^2$ term in the scaling factor is calculated as

$$\overline{DB}^2 = \overline{D}_{\perp} B_{\perp}^2 + \overline{D}_{\parallel} B_{\parallel}^2$$

where $\overline{D}_{\perp}$ is the component of the diffusion coefficient perpendicular to the platelets and $\overline{D}_{\parallel}$ is the component parallel to the platelets. The diffusion coefficient components are calculated with the equation

$$\overline{D}_k = \frac{\sum_n \sum_m V_n \Phi_n \frac{1}{\Sigma_{tr_m}} P_{nm,k}}{3 \sum_n V_n \Phi_n} \qquad (2.12)$$

where Σ_{tr_m} is the transport cross section in the $m^{\underline{th}}$ region and $P_{nm,k}$ are directional collision probabilities. These probabilities are related to the normal collision probabilities by

$$^1/3\ P_{nm,\perp} + {}^2/3\ P_{nm,\parallel} = P_{nm}$$

in infinite slab geometry. The diffusion coefficient, Eq. (2.12), was derived from integral transport theory by utilizing the mean square distance relation for the diffusion area. This procedure is equivalent to the results of Benoist /7/ if one neglects the angular correlation terms which are considered to be small in thin plate-type fast critical assemblies. For the collision probabilities in Eq. (2.12) the region optical thicknesses of the cell are calculated with the transport cross section rather than the total cross section. In this case one obtains the correct homogeneous limit of the diffusion coefficient in Eq. (2.12).

With the solution of the unit cell flux and self-shielded cross sections the KAPER program is able to generate homogenized cross sections

$$\overline{\Sigma}_x = \frac{\sum_m V_m \Phi_m \Sigma_{x_m}}{\sum_m V_m \Phi_m}$$

for use in a multidimensional homogeneous flux program to solve for the global parameters of the assembly.

3. Calculations within a Local Perturbation of the Unit Cell

In many instances measurements in a critical assembly involve a disturbance of the repeating unit cell of the assembly. For example, a portion of a cell may be removed for the insertion of a channel in which reaction rates are to

be measured with chambers, or in a reactivity worth measurement, a low density plate of inert material may be inserted between two plates of the cell at the position into which a sample is to be placed. In both of these cases the periodicity of the unit cell is disturbed. We shall call this cell containing the local perturbation, including the surrounding unit cells in which the flux is significantly disturbed by the perturbation, a perturbed cell. As this is a very practical problem of interest to the evaluators of experiments performed in critical assemblies a capability of solving for the flux, and therefore reaction rates, in such a situation was built into the KAPER program.

To find the flux and adjoint distribution in the perturbed cell it is assumed that the change in the assembly (introduction of the perturbed cell) is sufficiently small as to not affect the criticality of the assembly nor the spectrum several mean free paths from the perturbed cell position. With this assumption the flux and adjoint distribution in the perturbed cell can be obtained by solving the integral transport equation, Eq. (2.4), as a fixed source equation. The source is the first-flight leakage (uncollided neutrons) from the surrounding normal unit cells several mean free paths removed from the perturbation, or in the case of the adjoint equation, the importance a perturbed cell neutron has upon escaping from the perturbed cell.

To write the equation for this case it is sufficient to formulate the equation from physical processes. For example, Eq. (2.4) can be simply derived by equating the total collision density in a particular energy group and region to the sum of the contributions from all energy groups and regions from which it is possible for neutrons to come.

Let us draw imaginary boundaries around the perturbed cell of the assembly. We have located these imaginary boundaries, as a result of the definition of the perturbed cell given above, at a point where the equilibrium spectrum of the assembly is reestablished. From a previous calculation of the normal unit cell we have, therefore, the flux solution outside these imaginary boundaries. Setting up the collision density balance within the imaginary boundaries we have the contribution of those neutrons which always remain within the boundaries and those that come from outside. Due to the particular location of the imaginary boundaries there is no contribution to the collision density of neutrons that are leaving the perturbed cell and returning after one or more collisions as these are already included in the source coming from outside our boundaries. Our equation would then read as follows:

$$V_n \Sigma_{t_n}^g \phi_n^g = \sum_m P_{mn}^{+g} \sum_k \left[\Sigma_{s_m}^{k\to g} + \chi^g \nu\Sigma_{f_m}^k \right] V_m \phi_m^k + S_n^g \qquad (3.1)$$

where P_{mn}^+ is the probability a neutron from region m suffers its first collision in region n while remaining within our imaginary boundaries. The fluxes and cross sections explicitly written in Eq. (3.1) are defined for the regions that compose the perturbed cell. Therefore the first term on the right-hand side of Eq. (3.1) represents the contributions from within our imaginary boundaries and the second term (S_n^g) the contribution from outside the boundaries. The source term S_n^g has an appearance similar to the first term in Eq. (3.1) except that the collision probabilities have a different definition. We may write the source equation as

$$S_n^g = \sum_m \varepsilon_{mn}^g \sum_k \left[\Sigma_{s_m}^{k\to g} + \lambda\chi^g \nu\Sigma_{f_m}^k \right] V_m \phi_m^k \qquad (3.2)$$

where ε_{mn} is the probability that a neutron in a region m outside our imaginary boundaries suffers its first collision in a region n inside the boundaries. The cross sections and fluxes in Eq. (3.2) are defined for the normal unit cell and are available from a previous calculation. Therefore S_n^g can be calculated directly and used in Eq. (3.1) to solve for the flux within the perturbed cell (inside the imaginary boundaries).

The solution of both Eq. (3.1) and the corresponding adjoint equation are carried out by the power iteration method as briefly outlined in the previous section.

4. Heterogeneous Perturbation Calculation

For the calculation of heterogeneous reactivity worths perturbation theory is used. Perturbation theory offers an advantage for the calculation of small changes in a system; this being that the change in the system is expressed directly rather than being the difference of two nearly equal quantities as one would have by calculating the eigenvalue separately for the perturbed and unperturbed systems. Therefore the heterogeneous fluxes and cross sections, obtained as described in the previous sections, are used in a perturbation theory formulation of the integral transport theory equation to obtain reactivity worths of small changes introduced into the assembly core.

However, since the flux depression, or peaking, in the sample can be as important an effect as the self-shielding of the sample cross sections the exact form of the perturbation equation is utilized in the KAPER program rather than a first-order form as is commonly employed in perturbation programs. Therefore formulating the perturbation equation with the integral transport theory flux equation (representing the perturbed state) and the adjoint equation (representing the unperturbed state) one obtains

$$\rho = \frac{1}{D_\rho} \sum_g \sum_m V_m \, \Phi_m^{\prime g} \left[-\delta\Sigma_{t_m}^g \, \Phi_m^{+g} + \sum_n \sum_k \delta(\Sigma_{s_m}^{g\to k} \, P_{mn}^k) \, \Phi_n^{+k} \right. \\ \left. + \lambda \sum_n \sum_k \sum_j \delta(\chi_j^k \nu\Sigma_{f_{j_m}}^g \, P_{mn}^k) \, \Phi_n^{+k} \right] \tag{4.1}$$

where $\rho = -\delta\lambda/\lambda'$ and the region index summations are over all regions where the perturbation operators are non-zero. The perturbation operator, in general δN, is defined as $(N'-N)$ where the prime denotes the quantity defined in the perturbed state. In the perturbation equations we will represent the fission source as a sum of contributions (index j) from each fissionable isotope present. The denominator of Eq. (4.1) is

$$D_\rho = \lambda' \sum_g \sum_m V_m \, \Phi_m^{\prime g} \sum_j \nu\Sigma_{f_{j_m}}^{\prime g} \sum_k \sum_n \chi_j^{\prime k} \, \Phi_n^{+k} \, P_{mn}^{\prime k} \tag{4.2}$$

We may rewrite Eq. (4.1) if we use the following form of the perturbation operator:

$$\delta(\Sigma_m \, P_{mn}) = (\delta\Sigma_m) \, P_{mn} + (\delta P_{mn}) \Sigma_m^{\prime}$$

In addition, we may also use the relationship between the source importance function ψ_m^{+k} and the colliding neutron importance function ϕ_n^{+k}

$$\psi_m^{+k} = \sum_n P_{mn}^k \phi_n^{+k}.$$

Introducing these relationships into Eq. (4.1) we can write the results as, after some rearranging,

$$\rho = \frac{1}{D_\rho} \sum_g \sum_m V_m \phi_m^{'g} \left[-\delta\Sigma_{a_m}^g \phi_m^{+g} + \sum_k \delta\Sigma_{s_m}^{g\to k} (\psi_m^{+k} - \phi_m^{+g}) \right. \tag{4.3}$$

$$\left. + \lambda \sum_j \sum_k \delta(\chi_j^k \nu\Sigma_{f_j}^g)_m \psi_m^{+k} + \sum_k \sum_n (\Sigma_{s_m}^{'g\to k} + \lambda \sum_j \chi_j^{'k} \nu\Sigma_{f_j}^{'g})_m \delta P_{mn}^k \phi_n^{+k} \right]$$

where $\Sigma_{a_m}^g$ is the total absorption cross section in region m and energy group g.

This equation has a form that renders itself to easy physical interpretation. A source neutron, from a fission or scattering reaction, is weighted by the source importance function while a colliding neutron is weighted by the colliding neutron importance function. The last term in Eq. (4.3) accounts for diffusion effects.

The form utilized in the KAPER program is, however, slightly different than Eq. (4.3). We can rearrange the equation to obtain the following results

$$\rho = \frac{1}{D_\rho} \sum_g \sum_m V_m \phi_m^{'g} \left[-\delta\Sigma_{a_m}^g \psi_m^{+g} + \sum_k \delta\Sigma_{s_m}^{g\to k} (\psi_m^{+k} - \psi_m^{+g}) \right.$$

$$+ \lambda \sum_j \sum_k \delta(\chi_j^k \nu\Sigma_{f_j}^g)_m \psi_m^{+k} + \delta\Sigma_{t_m}^g (\psi_m^{+g} - \phi_m^{+g}) \tag{4.4}$$

$$\left. + \sum_k \sum_n (\Sigma_{s_m}^{'g\to k} + \lambda \sum_j \chi_j^{'k} \nu\Sigma_{f_j}^{'g})_m \delta P_{mn}^k \phi_n^{+k} \right]$$

The only advantage to Eq. (4.4) is that the first three terms can be identified as the normal absorption, scattering, and fission perturbation terms.

The perturbed flux in Eq. (4.4) is obtained with the procedure explained in Section 3. In this case the disturbance in the unit cell is the inserted reactivity sample. By utilizing Eq. (3.1) to find the flux in and around the sample one accounts also for the perturbation, due to the insertion of the sample, in the sample environment.

Since the KAPER program is a lattice program the denominator of Eq. (4.4) can not be calculated for the entire assembly core and reflector. The calculation of the denominator, or normalization integral as it is commonly called,

is best accomplished with a multidimensional flux program. Therefore the procedure selected for the calculation of the denominator is as follows

$$D_\rho = F(o) D_{NOR}$$

where

$$D_{NOR} = \frac{\lambda \sum_g \sum_m V_m \phi_m^g \sum_j \nu\Sigma_{f_{j_m}}^g \sum_k \sum_n \chi_j^k \phi_n^{+k} P_{mn}^k}{\sum_n V_n}$$

and

$$F(o) = \frac{\int d^3r \sum_j \sum_g \nu\Sigma_{f_j}^g(r) \psi^g(r) \sum_k \chi_j^k \psi^{+k}(r)}{\sum_j \sum_g \nu\Sigma_{f_j}^g \psi_{(o)}^g \sum_k \chi_j^k \psi_{(o)}^{+k}}$$

In these equations it is assumed that the effect of the reactivity sample in the calculation of the normalization integral is negligible. Therefore the perturbed fission source is replaced by its unperturbed value. For small-sample reactivity worth, for which the program is designed to handle, this approximate is quite valid.

The factor D_{NOR} is calculated for a normal assembly cell. F(o) is the normalization integral normalized by the neutron and importance source at the center of the assembly. The integration in F(o) is over the entire assembly core and reflector. This factor is obtained in an independent calculation, such as a two-dimensional diffusion calculation, and is used as input data to KAPER.

5. Numerical Results

In this section results of a number of various calculations are given which illustrate the versatility and validity of the methods utilized in the KAPER program. In some instances the results are compared to those of other computer programs and in other instances to direct experimental results. The results selected as illustrative examples depend primarily on the calculational model and only to a second order on the cross section data used.

5.1 Heterogeneity Calculations

To demonstrate the improvement of the methods used in KAPER over those in ZERA (see Section 2) a series of k_∞ calculations were performed for a cell similar to that of the SNEAK-5C assembly /8/. This was a null-reactivity assembly with a soft spectrum and strong heterogeneity effects. The core contained mainly mixed oxide and graphite.

The k_∞ values obtained for cells of different thicknesses are given in Table I. The following comments concerning the results can be made:

a) As expected from the theory, the results for the quasi-homogeneous case agree well.

b) The two codes, ZERA and KAPER, using the same approximation for the collision probabilities, give k_∞ values which differ by 0.6% for the full cell and less than that for the smaller cells. Thus the methods in the ZERA code may be used unless large heterogeneities are involved.

c) The k_∞ values before iteration on the source densities are given in brackets. The figures indicate that the changes due to the iteration are by one order of magnitude smaller than the difference in values given by the two codes. Therefore the iteration on the source is necessary only in cases of large heterogeneity.

The dependence of the heterogeneity effect on the background cross section, as used in the formulation of the effective resonance self-shielded cross section, is shown in Table II. Routinely the KAPER program uses the background cross sections of ^{238}U equal to its potential cross section (σ_{p8} = 10.6 barns) in the resonance groups. For comparison with ZERA calculations performed by Kiefhaber /9/, the background cross section of ^{238}U in KAPER was set equal to the total unshielded cross section σ_{t8}. Whereas the δk obtained by Kiefhaber with ZERA (Table II) depends strongly on the background cross section, this dependences is very weak in the KAPER results. In fact, the KAPER k_{HET} depends on the background cross section in much the same manner as k_{HOM} which is additional evidence for the conclusion that the approximations in the KAPER program are similar to the approximations used in homogeneous calculations. Furthermore, as the resonances of ^{238}U are strongly self-shielded, one would expect better results from ZERA by using σ_{p8} rather than σ_{t8} as a background cross section. This expectation is borne out by the results shown in Table I, where the ZERA δk is fairly close to the true KAPER δk.

The influence of the ^{238}U background cross section on the self-shielded cross section of ^{239}Pu is shown in Table III. Though the change in the background cross section is very large (σ_{t8} is certainly an extreme overestimate) the changes in the self-shielded cross sections are small, except in group 18. Thus it is demonstrated that the cross sections as defined in this paper are insensitive to the background cross sections.

5.2 Calculation of Cell Reaction Rates

In the hard spectrum core of SNEAK-7B /10/ studies were made on the effect of structural materials (stainless steel and aluminium) on spectral indices measured with foils. In addition, the measurement was designed to provide a verification check for the method used in KAPER to calculate the flux and reaction rate distribution in a local perturbation of the assembly core. The core of SNEAK-7B consisted of a simple unit cell of one mixed oxide platelet (uranium and plutonium) and one uranium oxide platelet. For the measurements uranium foils were placed between the normal platelets of the cell to serve as a reference. Additional foils were placed between stainless steel platelets, and aluminium platelets, of two thicknesses. This configuration is shown in Fig. 1. The addition of the stainless steel and aluminium represents a local perturbation in the normal repeating unit cell. The results of the KAPER calculations for this experiment are shown in Fig. 2. These results are given as the percent change in the spectral index σ_{c8}/σ_{f5} with respect to the reference measurement. The effect of the cross section set used in the calculation of the change of the spectral index was small ($\approx$10%), although not negligible. In general the agreement with the experimental results is quite good.

As an illustration of the calculation of cell reaction rate fine structures the results of a measurement and calculation are shown in Fig. 3. In this figure the cell composition is shown along the ordinate axis. The assembly for this

measurement was a uranium null-reactivity core. Shown in Fig. 3 is the calculated cell fine structure of ^{238}U fission along with results of uranium foil measurements. The fine structure of the cell is slightly overestimated by KAPER. These results are fairly representative of the agreement in a wide range of measurements.

5.3 Analysis of Reactivity Worth Measurements

A series of small-sample reactivity worth measurements performed in SNEAK have been analyzed with the methods described in this paper. These include measurements performed in SNEAK-5C /8/. The assembly 5C of SNEAK was a null-reactivity core with a soft spectrum and strong heterogeneity effects as explained previously. The sample reactivity measurements were performed in two positions within the unit cell of the core as shown in Fig. 4.

For comparison with experiment the ratio of the sample worth in position 1 to that in position 2 is used. This eliminates the uncertainty associated with β_{eff} and the absolute magnitude of the normalization integral. The results of these calculations are given in Table IV. This is quite clearly an example of where first order homogeneous perturbation, as normally used to interpret these types of measurements, fails. The measurements, in this assembly, are extremely position dependent and must be, therefore, interpreted with a program having the capabilities of KAPER. Except for the ^{240}Pu sample the calculated and measured reactivity worth ratios agree within the experimental errors. The calculation of the sample size effect of the ^{238}U samples, for the two measurement positions, is shown in Fig. 5. It is seen that the program slightly underpredicts the sample size effect.

5.4 Utilization of Cell Homogenized Cross Sections

The importance of correctly calculating cross sections for the heterogeneous assembly is illustrated in the following example. In an experiment to study the effect of leakage in an axial sodium void traverse the platelets of the assembly in the voided region were oriented first, parallel to the direction of the traverse, and second, perpendicular to the traverse direction. To analyze the experiment one-dimensional diffusion theory perturbation theory was used. The cross sections for the one-dimensional calculation were generated by a routine at Karlsruhe which calculates self-shielded cross sections using the f-factor concept for homogeneous media. In addition, the KAPER program was used to calculate homogenized cross sections for the heterogeneous cell of the assembly. For the two different platelet orientations the diffusion coefficient was set equal to its component parallel to the platelets, and to its component perpendicular to the platelets, for the respective cases. The results of using these cross sections in the one-dimensional diffusion calculation are shown in Fig. 6. The use of the homogenized cross sections significantly lowers the calculated curve. The effect of the leakage in the two different platelet orientations is quite nicely described by the diffusion coefficients calculated by KAPER.

6. Conclusions

It has been demonstrated that the methods employed in the KAPER program are extremely useful for the analysis of measurements performed in a heterogeneous environment of fast critical assemblies. The application of the

f-factor concept is not as accurate as the methods used in ultrafine group slowing-down codes; nevertheless the procedure certainly yields sufficient accuracy, with a tremendous savings in computer time, for routine calculations.

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Table I k_∞ for the SNEAK-5C Simplified Cell

	ZERA		KAPER	
Relative Thickness of the cell	k_∞	δk	k_∞	δk
10^{-3} (quasi homogeneous)	0.9342	--	0.9343	---
1/4	0.9640	0.0298	0.9627 (0.9628)+	0.0284
1/2	0.9849	0.0507	0.9828 (0.9825)	0.0485
Full	1.0156	0.0814	1.0101 (1.0094)	0.0758

+) k_∞ values in parentheses are values before iteration on the source densities

Table II Dependence of k_∞ on the background cross section of ^{238}U

	SNEAK-5C, ZERA /4/			Simplified SNEAK-5C, KAPER		
	k_{HOM}	k_{HET}	δk	k_{HOM}	k_{HET}	δk
Self-shielded with σ_{p8}	0.9340	1.0016	+0.0676	0.9343	1.0101	0.0758
Self-shielded with σ_{t8}	0.9404	0.9504	+0.0100	0.9414	1.0211	0.0797

k_{HOM} is defined as k_∞ of the quasi-homogeneous cell wherein the cell thickness is multiplied by 10^{-3}, and k_{HET} is defined as k_∞ of the full cell.

Table III Dependence of the effective cross sections of ^{239}Pu on the background cross section of ^{238}U (KAPER) (SNEAK-5C simplified cell, region 5)

	Background cross section of ^{238}U, b	Self-shielded cross sections of ^{239}Pu			
		σ_{f9}	% difference	σ_{c9}	% difference
Group 14 (1.00 - 2.15 keV)					
Infinite Dilution	-	3.929		2.324	
Self-shielded with σ_{p8}	10.6	3.778	-3.8	2.192	-5.7
Self-shielded with σ_{t8}	19.9	3.794	+0.4	2.206	+0.6
Group 16 (215-465 eV)					
Infinite Dilution	-	12.48	-	8.63	
Self-shielded with σ_{p8}	10.6	10.91	-12.8	6.72	-22.1
Self-shielded with σ_{t8}	20.3	11.06	+1.4	6.87	+2.2
Group 18 (46.5-100 eV)					
Infinite Dilution	-	54.5	-	50.8	
Self-shielded with σ_{p8}	10.6	31.8	-42	21.6	-57
Self-shielded with σ_{t8}	40.2	34.0	+ 7	23.9	+10

Table IV Reactivity Worth Ratios in SNEAK-5C

Position 1 / Position 2	Sample Weight [g]	Experiment	Calculation (KAPER)
^{239}Pu	5	1.135±0.019	1.146
^{238}U	5	3.440±0.430	3.127
^{238}U	60	1.545±0.251	1.540
^{240}Pu	3	1.635±0.092	1.310
Fe_2O_3	3	0.440±0.109	.430

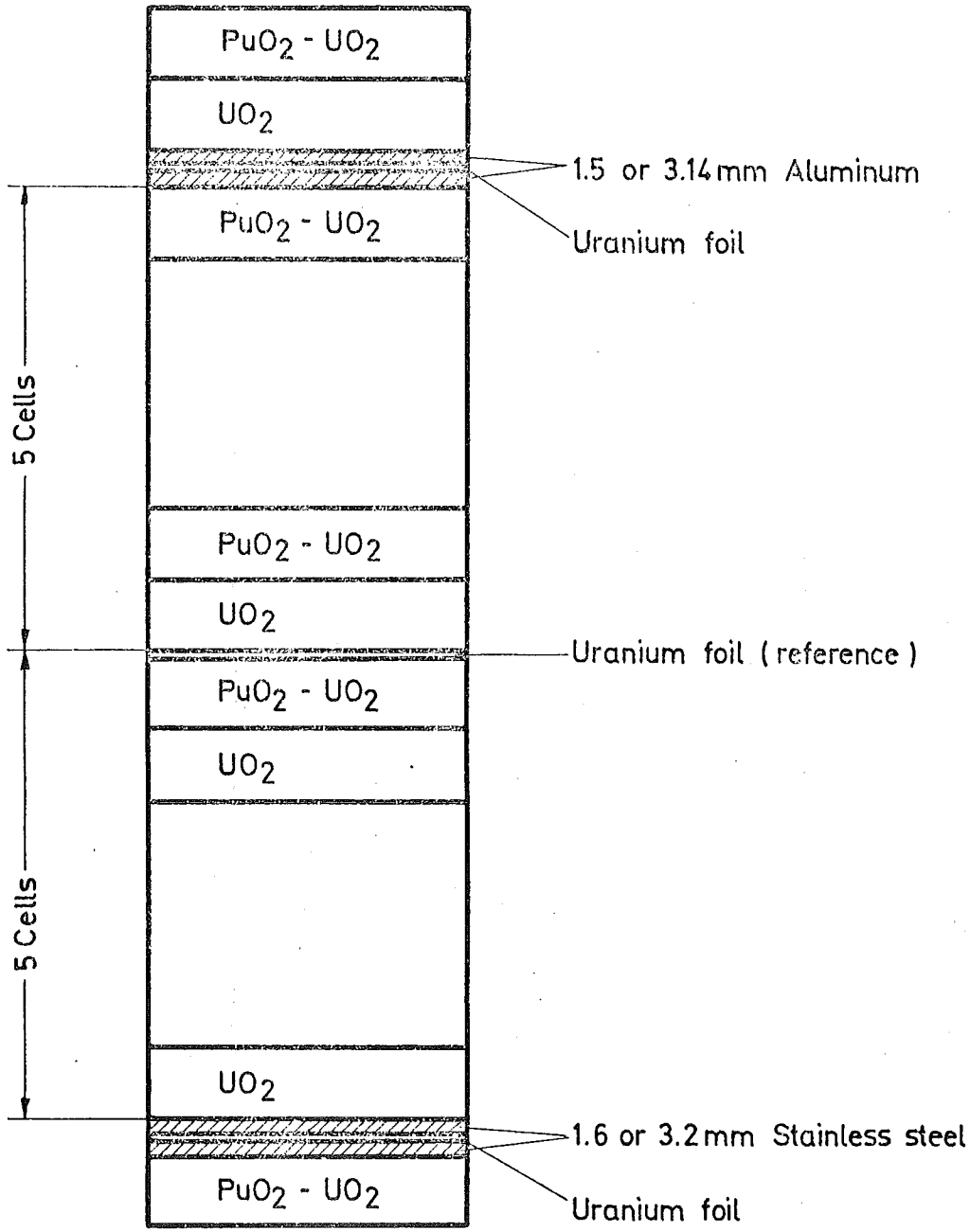

Fig.1 Spectral indices measurements in SNEAK-7B

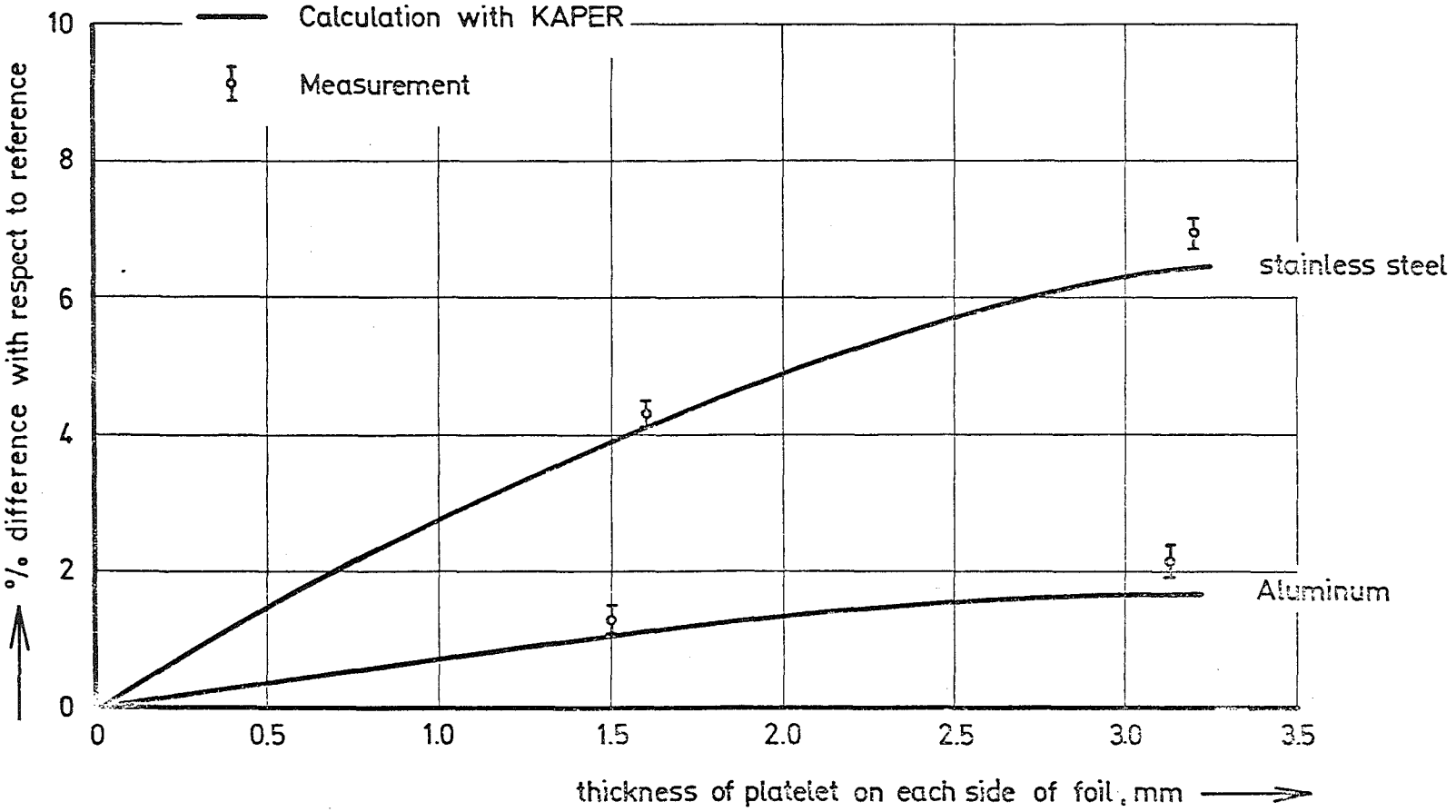

Fig.2 Change in σ_c^8 / σ_f^5 as function of the thickness of material surrounding foil, SNEAK - 7B

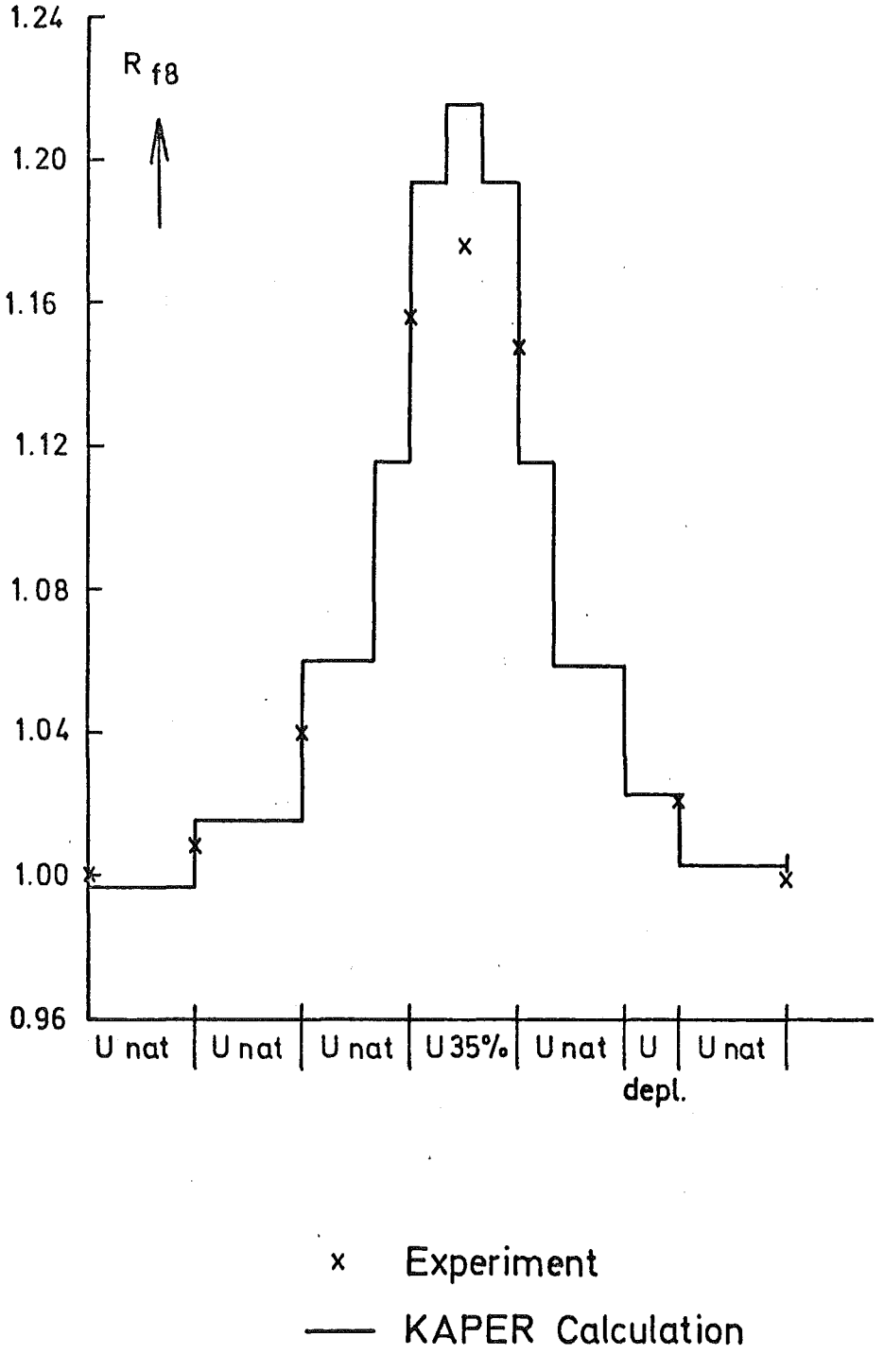

Fig. 3 Fine structure of fission rate R_{f8} in SNEAK-8Z

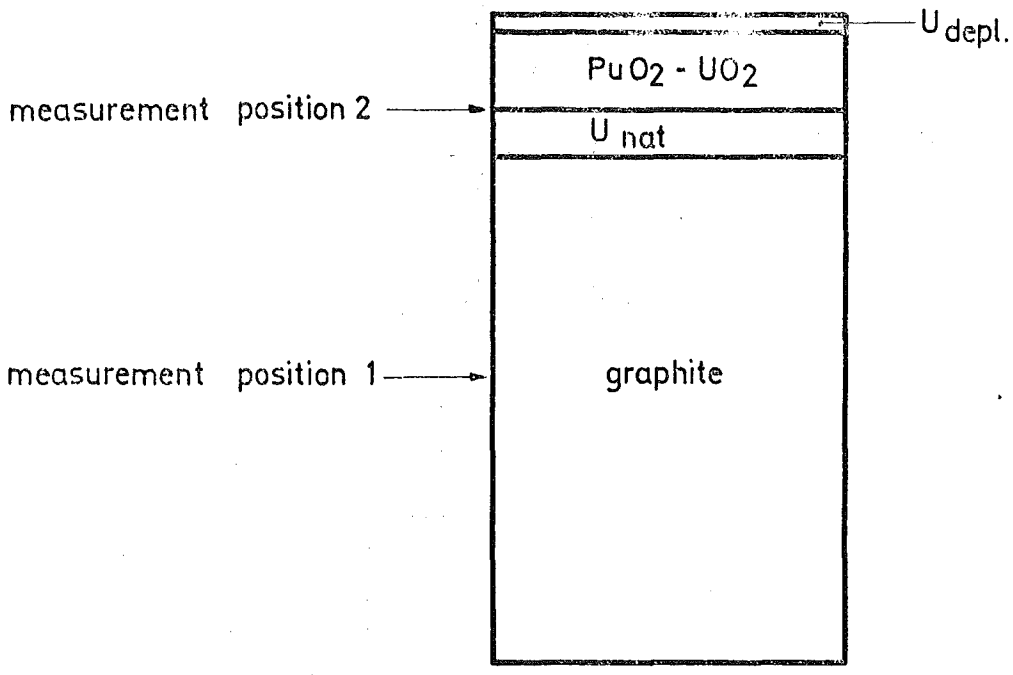

Fig.4 Principal cell structure of SNEAK-5C

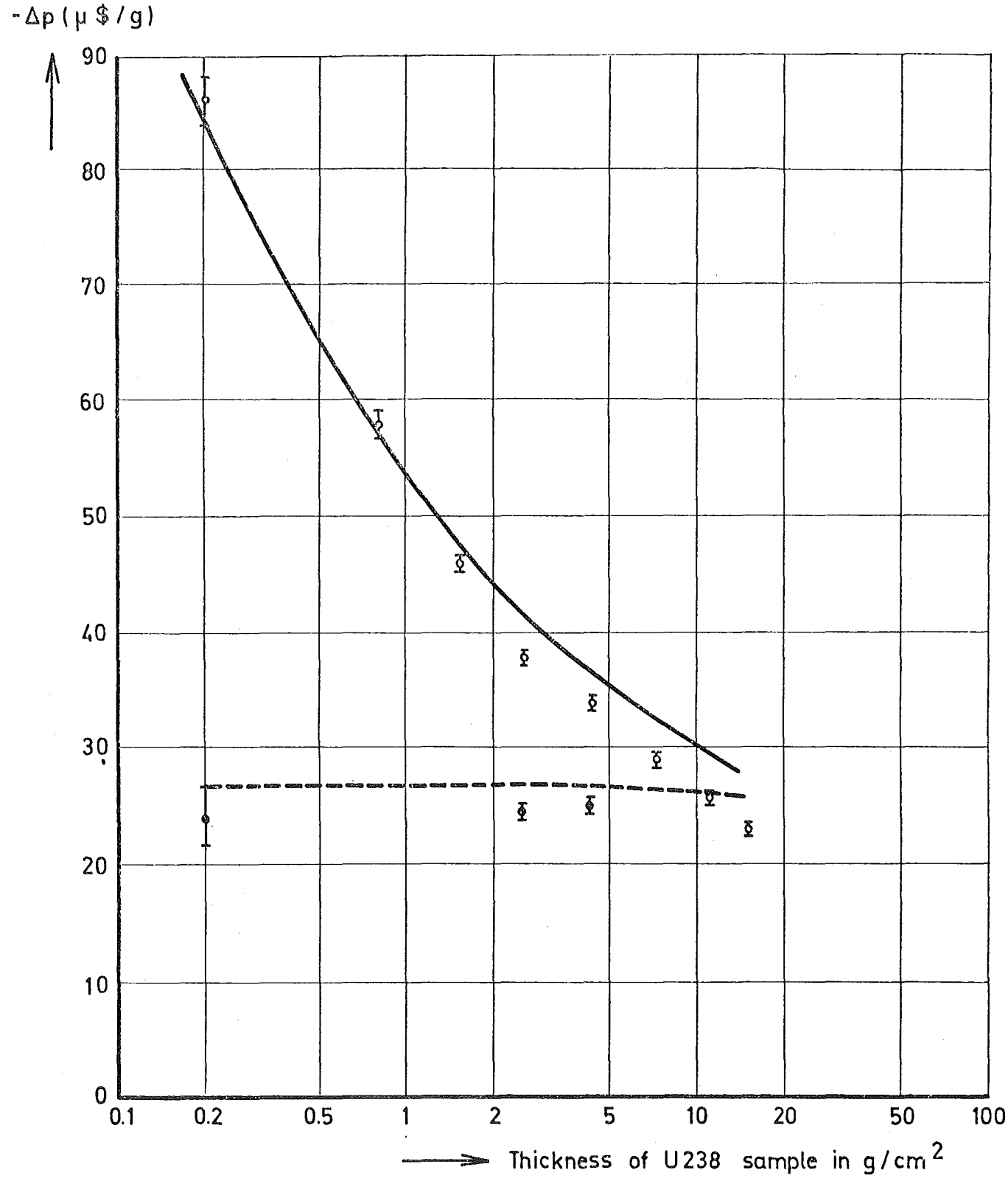

Fig.5 Central Reactivity Worth of U238 in SNEAK-5C

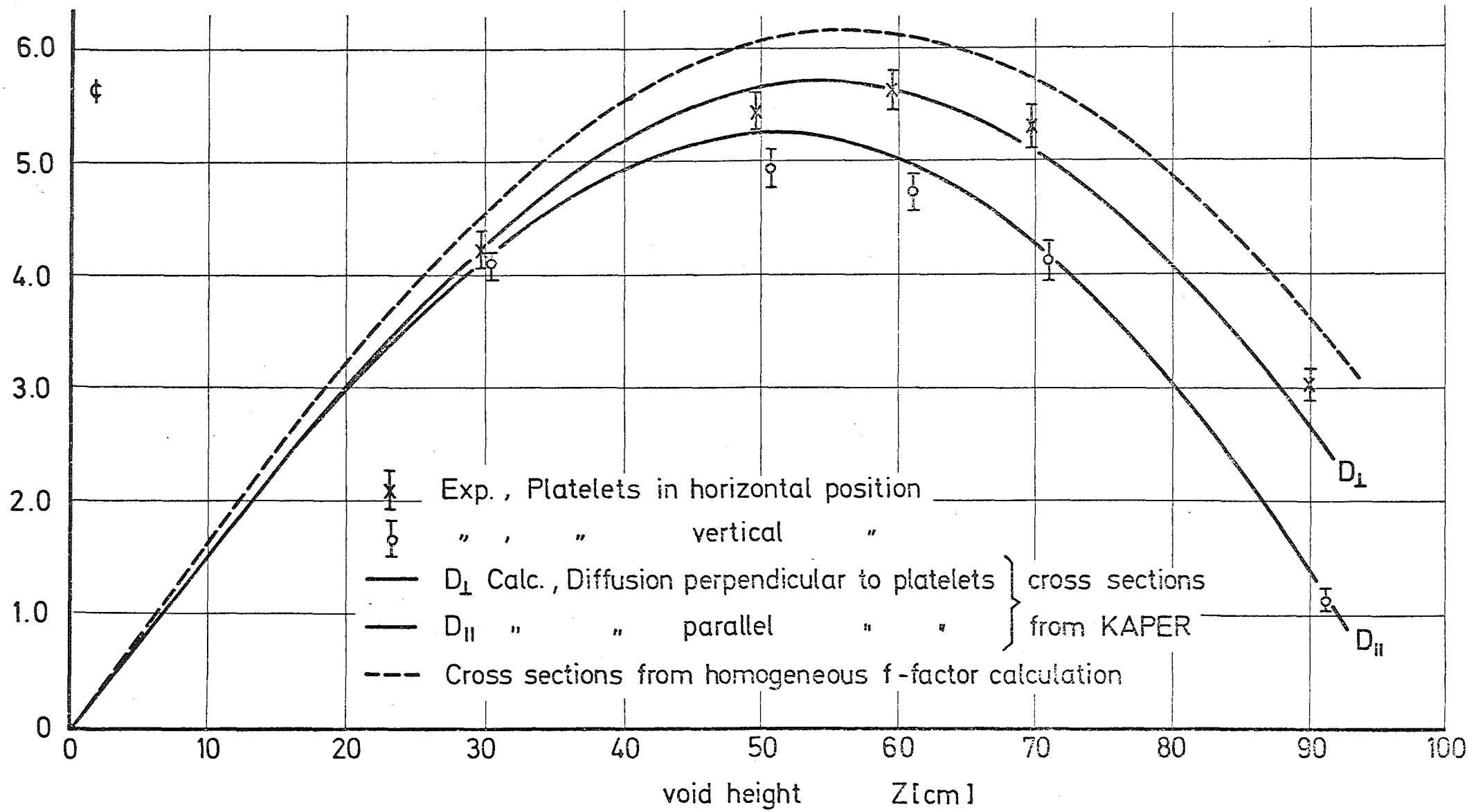

Fig. 6 Integrated axial sodium void reactivity effect for different platelet orientations, SNEAK-9B

VII. Cross Section Library and Isotope Name Convention

Use outside of Karlsruhe NUSYS system

The KAPER program was designed to function within the NUSYS program system of Karlsruhe. Therefore the program reads the required cross section data directly from the prepared cross section data units of NUSYS with the two subroutines GRREAP and GROOCP. Therefore, built into the program was a certain isotope identification convention and the established energy group structure containing 26 groups. To use the program outside of the Karlsruhe NUSYS program system a new subroutine GRREAP is provided. A listing of this short subprogram is included in the following. The data and format required by the program are explained in the FORTRAN listing. The cross sections and their respective self-shielding factors can be generated from ENDF data, or similar data files, by a number of available programs, for example ETOX or IDX from the Argonne Computer Code Center (see Ref. /3/).

Number of energy groups

To calculate with more than 26 energy groups it is only necessary to change the common block /CH/ which contains the prepared fission neutron spectra for the fissionable isotopes. This common block is contained in subroutines PPM760, NSPEK, SPEK, PPM761 and in BLOCK DATA. The rest of the program is variably dimensioned for the number of energy groups. No change in common block /CH/ is necessary if one calculates with less than 26 groups.

Isotope name convention

In assigning fission neutron spectra to the various fissionable isotopes encountered within a given problem the program searches the isotope lists for recognizable fissionable isotopes. For this purpose the isotopes recognized by the program and assigned the correct fission neutron spectrum are the following:

^{232}Th	-	TH320
^{233}U	-	U2330
^{234}U	-	U2340
^{235}U	-	U2350, U_5A0, U_5B0
^{236}U	-	U2360
^{238}U	-	U2380, U_8A0, U_8B0
^{239}Pu	-	PU390, PU0B0, PU2B0, PU9A0, PU9B0
^{240}Pu	-	PU400
^{241}Pu	-	PU410
^{242}Pu	-	PU420

The several possibilities for the isotopes ^{235}U, ^{238}U, and ^{239}Pu allow for the inclusion of several cross section data sets for the same isotope, but differing in their respective temperatures (Doppler broading of the cross sections). However when assigning a fission neutron spectrum to a particular isotope using the input option on cards K10 and K11 of phase 99999 the program only

recognizes the first identification of the isotope as given in the list above or as spelled out on card K10 of phase 99999. Therefore on the input cards K5 and K6 all possible combinations above may be used, but on input cards K10 only the first given isotope identification name given above may be used.

The energy group limits for the 26 group structure used to generate the built in fission neutron spectra from the Maxwellian distribution, given on page 6, are shown in the following table.

Group	Upper Energy Limit (ev)	Δu
1	10.5×10^6	0.48
2	6.5×10^6	0.48
3	4.0×10^6	0.48
4	2.5×10^6	0.57
5	1.4×10^6	0.57
6	8.0×10^5	0.69
7	4.0×10^5	0.69
8	2.0×10^5	0.69
9	1.0×10^5	0.77
10	4.65×10^4	0.77
11	2.15×10^4	0.77
12	1.0×10^4	0.77
13	4.65×10^3	0.77
14	2.15×10^3	0.77
15	1.0×10^3	0.77
16	4.65×10^2	0.77
17	2.15×10^2	0.77
18	1.0×10^2	0.77
19	46.5	0.77
20	21.5	0.77
21	10.0	0.77
22	4.65	0.77
23	2.15	0.77
24	1.0	0.77
25	0.465	0.77
26	0.215	0.77

In the generation of the fission neutron spectra the assumption used in the KAPER program are that neutrons emitted above the upper energy limit of the first group are included in the first group and all neutrons emitted below 10 keV are included in the group containing that energy point. These spectra, as included in KAPER, for the different temperatures which characterize the various fissionable isotopes are shown below.

Temperatures (MeV)

Group	1.30	1.31	1.32	1.34	1.35	1.39	1.41
1	0.018609	0.019285	0.01995	0.021233	0.02194	0.025134	0.02656
2	0.08579	0.0873	0.0888	0.09179	0.09328	0.09918	0.1021
3	0.1742	0.1754	0.1766	0.1789	0.1800	0.1842	0.1862
4	0.2625	0.2624	0.2623	0.2621	0.2619	0.2610	0.2605
5	0.2045	0.2035	0.2025	0.2004	0.1994	0.1953	0.1933
6	0.1473	0.1461	0.1449	0.1427	0.1416	0.1372	0.1352
7	0.06567	0.06504	0.06441	0.06319	0.06260	0.0603	0.05921
8	0.0261	0.02582	0.02555	0.02502	0.02477	0.02378	0.02331
9	0.01035	0.01023	0.01012	0.009904	0.009799	0.009394	0.009201
10	0.003397	0.003359	0.003321	0.003249	0.003213	0.003078	0.003014
11	0.001584	0.001566	0.001549	0.001514	0.001498	0.001434	0.001404
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0
↓							
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
      SUBROUTINE GRREAD (GRSN,SNOG,Q,SMTOT,ISZ,NOG,IQ,FSTF)
C
C*** PROGRAM TO READ CROSS SECTIONS FROM LIBRARY FOR KAPER
C*** FOR USE OUTSIDE OF THE KARLSRUHE NUSYS PROGRAM SYSTEM
C
      REAL*8 ISOT(20),GRSN(3),TYP,ATEXT(60),BTEXT(50),ISFT,ISON(20),ISO
      DIMENSION SNOG(7,ISZ,NOG),Q(ISZ,4,IQ),SMTOT(ISZ,NOG,NOG),
     X    JTS(20),FSTF(NOG,20)
      COMMON ATEXT,ISOT,ISON,BTEXT,K360(50)
      COMMON /M10760/ N(3),NG,M(8),NIS
C
      INF=0
      NSF=4
      REWIND NSF
      PRINT 2002
 2002 FORMAT(//' ***CROSS SECTION DATA FROM SPECIAL LIBRARY***')
      DO 100 IS=1,ISZ
  100 JTS(IS)=0
      IGZ=8*NOG
C
C********** EXPLANATION OF CROSS SECTION DATA REQUIRED FROM LIBRARY *****
C                    FOUR RECORDS REQUIRED FOR EACH ISOTOPE
C
C-----------------------------------------------------------------------
C*******************************RECORD 1********************************
C-----------------------------------------------------------------------
C         ISO IS A REAL*8 IDENTIFICATION OF ISOTOPE, FOR EXAMPLE U2380
C-----------------------------------------------------------------------
C*******************************RECORD 2********************************
C-----------------------------------------------------------------------
C                  Q(IS,J,L) MATRIX, IS = ISOTOPE INDEX
C-----------------------------------------------------------------------
C                              L=1 TO NOG,
C          THE ENERGY GROUP DEPENDENT VALUES OF THE FOLLOWING CROSS
C          SECTIONS, WHERE NOG IS THE NUMBER OF ENERGY GROUPS
C-----------------------------------------------------------------------
C         J=1,  Q=NU*SIGMA-FISSION (INFINITE DILUTION)
C         J=2,  Q=SIGMA-ABSORPTION (INFINITE DILUTION)
C         J=3,  Q=SIGMA-ELASTIC SCATTERING (INFINITE DILUTION)
C         J=4,  Q=SIGMA-TRANSPORT (INFINITE DILUTION)
C-----------------------------------------------------------------------
C                               L=NOG+1 TO 8*NOG
C-----------------------------------------------------------------------
C     SELF-SHIELDING FACTORS FOR THE RESPECTIVE CROSS SECTIONS J=1 TO 4
C     FOR VARIOUS BACKGROUND CROSS SECTIONS
C         L=NOG+1 TO 2*NOG,    Q=F(SIGMA-BACKGROUND=0.0)
C         L=2*NOG+1 TO 3*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+1)
C         L=3*NOG+1 TO 4*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+2)
C         L=4*NOG+1 TO 5*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+3)
C         L=5*NOG+1 TO 6*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+4)
C         L=6*NOG+1 TO 7*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+5)
C         L=7*NOG+1 TO 8*NOG,  Q=F(SIGMA-BACKGROUND=1.0E+6)
C-----------------------------------------------------------------------
C*******************************RECORD 3********************************
C-----------------------------------------------------------------------
C      SNOG(I,IS,IG) MATRIX, IG = ENERGY GROUP INDEX, IS = ISOTOPE INDEX
C-----------------------------------------------------------------------
C         I=1, SNOG=SIGMA-TOTAL (INFINITE DILUTION)
C         I=2, SNOG=SIGMA-TRANSPORT (INFINITE DILUTION)
```

```
C          I=3,  SNOG=SIGMA-INELASTIC SCATTERING PLUS SIGMA-(N,2N)
C          I=4,  SNOG=SIGMA-ELASTIC REMOVAL
C          I=5,  SNOG=MU (AVERAGE COSINE OF THE ELASTIC SCATTERING ANGLE)
C          I=6,  SNOG=NU (NUMBER OF NEUTRONS PER FISSION)
C          I=7,  SNOG=SIGMA-TOTAL GROUP REMOVAL (INFINITE DILUTION)
C-----------------------------------------------------------------------
C     FSTF(IG,IS) MATRIX, IG = ENERGY GROUP INDEX, IS = ISOTOPE INDEX
C-----------------------------------------------------------------------
C              FSTF=TOTAL CROSS SECTION SELF-SHIELDING FACTOR FOR
C                   BACKGROUND CROSS SECTION EQUAL ZERO
C-----------------------------------------------------------------------
C*************************************RECORD 4*****************************
C-----------------------------------------------------------------------
C          SMTOT(IS,JG,IG) MATRIX, IG AND JG ARE ENERGY GROUP INDICES,
C               AND IS = ISOTOPE INDEX
C-----------------------------------------------------------------------
C       SMTOT(IS,JG,IG)=SIGMA-INELASTIC SCATTERING MATRIX PLUS
C                       2.0*SIGMA-(N,2N) MATRIX FROM GROUP IG TO JG
C-----------------------------------------------------------------------
C
   99 CONTINUE
      READ(NSF,END=1010)ISO
      DO 110 IS=1,ISZ
      IF(ISO.EQ.ISOT(IS)) GO TO 120
  110 CONTINUE
      READ(NSF)
      READ(NSF)
      READ(NSF)
      GO TO 99
  120 IND=IND+1
      JTS(IND)=IS
      READ(NSF)  ((Q(IS,J,L),J=1,4),L=1,IGZ)
      READ(NSF) ((SNOG(I,IS,IG),I=1,7),IG=1,NOG),(FSTF(IG,IS),IG=1,NGG)
      READ(NSF) ((SMTOT(IS,JG,IG),JG=1,NGG),IG=1,NOG)
      DO 200 IG=1,NGG
      SUM=0.
      DO 170 JG=1,NOG
  170 SUM=SUM+SMTOT(IS,JG,IG)
      SMTOT(IS,IG,IG)=SNOG(7,IS,IG)-SUM-Q(IS,2,IG)-SNOG(4,IS,IG)
     X     +SMTOT(IS,IG,IG)
  200 CONTINUE
      GO TO 99
 1010 IF(IND.EQ.ISZ)GO TO 250
      PRINT 2004
 2004 FORMAT(//' ***NOT ALL OF THE ISOTOPES REQUESTED ARE FOUND IN THE L
     XIBRARY***')
      DO 260 I=1,ISZ
      DO 265 K=1,IND
      IF(JTS(K).EQ.I)GO TO 270
  265 CONTINUE
      PRINT 2005,ISOT(I)
 2005 FORMAT(/,' ISOTOPE NOT FOUND IS',2X,A8)
  270 CONTINUE
  260 CONTINUE
      PRINT 2006
 2006 FORMAT(//' ***PROGRAM STOP***')
      STOP
  250 RETURN
      END
```

VIII. References

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