# The Fast Reactor Cell Code KAPER 4

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Abstract

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This report describes the code KAPER4, a multigroup
code for neutronics calculations of heterogeneous
lattices of fast reactors. The code solves the integral
transport equation with isotropic scattering by a
collision probability formalism. Though restricted to
one dimension, the code can handle both pin cells of
a fast reactor, and plate cells of heterogeneous criti-
cal facilities.

The method, including the treatment of resonance self-
shielding based on the f-factor concept, is explained
in detail. A description of the program structure and
an input description are given.
The code calculates eigenvalues, fluxes, and reaction
rates. It has several additional capabilities, which
are also described.

Zusammenfassung

## Der Zell-Code KAPER4 für Schnelle Reaktoren

In diesem Bericht wird KAPER4 beschrieben, ein Multigruppen-
Neutronik-Code zur Berechnung von Zellgittern Schneller Reak-
toren. Der Code löst die integrale Transportgleichung mit iso-
troper Streuung nach einem Stoßwahrscheinlichkeitsverfahren.
Obwohl auf eindimensionale Probleme beschränkt, kann der Code
sowohl Stabzellen schneller Leistungsreaktoren als auch Plätt-
chenzellen kritischer Nullenergieanordnungen behandeln.

Die Methode, die eine Behandlung der Resonanzselbstabschirmung
auf der Basis des f-Faktor-Konzeptes einschließt, wird ausführ-
lich erläutert. Eine Beschreibung der Programmstrukturen und
der Eingabe wird ebenfalls gegeben.

Der Code berechnet Eigenwerte, Flüsse und Reaktionsraten.
Darüber hinausgehende Optionen sind zusätzlich möglich. Sie
werden im Detail beschrieben.

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## 1. Introduction

The code KAPER4 calculates eigenvalues and fluxes for heteroge-
neous plate or pin cells of fast reactor lattices. It is an exten-
sion of the earlier code KAPER /1/, which is not used any more.

Cell heterogeneity effects in fast reactors are much smaller than
in thermal reactors, and can be neglected in many cases, e.g. for
survey or scoping type calculations. For example, in a sodium-
cooled power reactor of the SNR-type, the cell thickness is $\lesssim 1$ cm,
as compared to the neutron mean free path $\gtrsim 5$ cm. The difference
in the multiplication factor due to this heterogeneity is only
of the order of 0.1 to 0.2%.
On the other hand, cell calculations are state of the art, and for
any more refined calculations, heterogeneity effects must be in-
cluded. Besides, there are configurations where heterogeneity is
more pronounced than in a standard SNR-type reactor, and cell
calculations are therefore mandatory:

- In plate-type fast critical assemblies, such as in
  SNEAK, the mean optical cell thickness is usually larger
  than in a power reactor, and fine structure effects are
  more pronounced. Flux variations in the cell are usually
  several percent. Refined experimental techniques were
  developed to measure e.g. reaction rates inside the fuel
  plates, or to place material worth samples between plates
  of a cell. These experiments can only be meaningfully
  analyzed with a cell code, and KAPER4 has special features
  to treat these configurations. In addition, KAPER4 is
  needed to correct for the different heterogeneity when
  critical assembly results are used for power reactor
  design.

- In the sodium-void case of a power reactor, or a sodium-
  void experiment in a fast critical assembly, the neutron
  streaming in the voided channels leads to an enhanced
  leakage, which is significant enough to necessitate a

heterogeneous treatment. Furthermore, the hetero-
geneous void case should be compared for consistency
with a heterogeneous "sodium-in" calculation to
determine the sodium-void reactivity effect.

The present version of KAPER4 can handle plate and pin-geometry,
but it is restricted to these one-dimensional cases. A more
accurate modelling of the cells, including e.g. subassembly cans,
would require collision probability routines in two or even three
dimensions, which are not available for KAPER4. Thus, configu-
rations like pin in a subassembly hexcan, mixed-pin cells in
critical experiments, or the single absorber rodlets in a control
rod, cannot be treated explicitly in KAPER4. However, in view
of the present effort to develop a European common cell code,
with the major activity going on in the United Kingdom and
in France, it is not planned to put any more effort into KAPER
development. Therefore, it is expected that the present status,
which is described in this report, will still be valid in the
future.

## 2. General Features, Capabilities and Limitations

KAPER4 is a broad-group cell code which solves the integral
transport equation with isotropic scattering in a collision
probability formalism. The buckling method is used to separate
the macroscopic reactor flux, and the microscopic cell flux.
The code performs zero-dimensional eigenvalue calculations with
given group- and direction dependent bucklings. This calculation
also provides fluxes or adjoint fluxes, and reaction rates in
the cell. In addition, KAPER4 produces cell-averaged cross
sections, as well as anisotropic diffusion coefficients
obtained by the method of Benoist. These cross sections can be
stored in the SIGMN block in the KAPROS system, and used
in whole-core calculations.

The code has its own cross section preparation routine. It reads
the data from a broad-group library, which also contains tabu-
lated self-shielding factors("f-factors"). The most frequently
used cross section set is KFKINR, which has 26 energy groups.
Self-shielding is then calculated by means of a procedure ori-
ginally due to Wintzer /2/, which can be considered as an extension
of Wigner's equivalence principle.
The flux calculation uses exclusively macroscopic cross sections
obtained by the KAPER cross section preparation routine.
Input of macroscopic cross sections is not possible.
The self-shielding calculation is not congruent with the one
used in the GRUCAL routine, which is considered standard for
a homogeneous case. Therefore, to keep GRUCAL as a basis, the
following procedure is generally used to prepare heterogeneous
cross sections: A GRUCAL run is carried out. In addition, KAPER4
is run for the heterogeneous cell, and also for the homogeneous
composition with averaged atom densities. The difference between
the cross sections produced by the two KAPER runs is added to
the GRUCAL cross sections. With this "difference method", the
different KAPER self-shielding procedure affects only the actual
"heterogeneity correction". To avoid this situation, one
would have to introduce subgroup data instead of tabulated

self-shielding factors.

In the flux calculation routine, the collision probabilities are calculated with the total cross sections; in some cases, it would be more appropriate to use the transport cross section (see section 6.2). The collision probabilities which are used to obtain the cell diffusion coefficients are, of course, calculated with the transport cross sections.

The transport cross sections produced by KAPER4 are flux-weighted over energy within an energy group. For whole core calculations, current-weighted transport cross sections are generally required, and produced by the GRUCAL code. This is again a reason to use the "difference method" to produce approximate values for the effective cell transport cross section. In general, this method can be used in good approximation because the difference between the two weightings is not large, provided the self-shielding factors were derived in a  consistent manner from the nuclear data base. Note, however, that some of the f-factors in the frequently used KFKINR group constant set are not consistent; the f-factors for the transport cross sections were not obtained from the same nuclear data base as those for the reaction cross sections.

## 3. Equations Used by the KAPER4 Code

### 3.1 Basic Method

KAPER4 solves the collision probability equations for periodic
lattices composed of plate or pin cells. These equations are
based on the integral transport equation with isotropic scattering.
The buckling method is used to separate the microscopic cell
flux and the global macroscopic flux distribution in the reactor.
The derivation of the KAPER4 equations will be outlined here,
and the approximations made in this derivation will be discussed.
Note that in the last decade, several different ways to define
cell-averaged quantities (cross section, cell diffusion coeffi-
cients) were proposed in the literature; some authors point out
that there is a certain arbitrariness in the definitions, and
they summarize the relative merits and drawbacks of them /3,4/.
This discussion will not be repeated here. Instead, we follow
the observation in /5/, that there is a unique way of defining
cell-averaged quantities which preserves the true reaction rates,
the leakage rate out of the cell, and, of course, also the eigen-
value. Thus, the arbitrariness in the definition comes in only
when one has to decide on which kind of approximation to this
"exact" definition should be used. It seems clear that for
fast reactors, where the total heterogeneity effect is usually
small, higher-order corrections to this heterogeneity effect are
completely negligible. Thus, it is sufficient to use a low-order
approximation. It turns out that the KAPER equations, which were
developed already in 1972 /1/, represent indeed such an approxi-
mation, which is, however, completely adequate for fast reactor
cells.
For simplicity, the following derivation is carried out for
the monoenergetic equation, for a medium without scattering,
but with a given isotropic source density Q(r) /6/. Later on,
it is straightforward to identify the source density as the sum
of fission neutron source, scattering source, and a potential
external source. In addition, the extension to the energy-dependent
case is also straightforward.

The monoenergetic transport equation reads

$$\Omega \; grad \; \psi(r, \Omega) + \Sigma \psi(r, \Omega) = \frac{1}{4\pi} \, Q(r) \qquad (3.1)$$

where $\psi(r, \Omega)$ is the angular neutron flux, and $\Sigma$ is the total cross section; in the case of no scattering, this is also the absorption cross section. The scalar flux and the neutron current are then defined by

$$\phi(r) = \int \psi(r, \Omega) \, d\Omega \; , \quad J = \int \psi \, \Omega \, d\Omega$$

The integration of eq.(3.1) over angle gives, if one observes that the first term can be written $div(\Omega\psi)$,

$$div \; J + \Sigma \phi = Q \qquad (3.2)$$

This is the differential neutron balance equation.
It is known from transport theory /6,7/ that the integral transport equation,

$$\phi(r) = \int d^3r' \, p(r', r) \, Q(r') \qquad (3.3)$$

is equivalent to the differential equation (3.1). p(r'r) is the probability that a neutron born at r' collides (and is absorbed) at r.
In addition, one can write a similar equation for the neutron current

$$J(r) = \int d^3r' \, P(r', r) \, Q(r') \qquad (3.4)$$

where P(r',r) is the current at r due to a unit source density at r' . Explicit expressions for p(r',r) and P(r',r) are given e.g. in /6/.

The separation into microscopic and macroscopic flux is per-
formed using the buckling method (see e.g. /5/), which is
based on the assumptions

- the periodic lattice (which may be a plate or pin lattice)
  extends to infinity in space

- the source density has the following space dependence

$$Q(r) = q(r) \exp(i \vec{B} \vec{r}) \tag{3.5}$$

where q(r) has the periodicity of the lattice, and the
vector $\vec{B}$ has components $B_x$, $B_y$, $B_z$, which are the square
roots of the bucklings in the three space dimensions.

One can now factorize the flux φ(r) by the definition

$$\phi(r) = \varphi(r) \exp(i \vec{B} \vec{r})$$

and arrives at the following integral equation for

$$\varphi(r) = \int d^3 r' \, p(r', r) \, q(r') \exp(i \vec{B}(\vec{r}' - \vec{r})) \tag{3.6}$$

As the exponential term in (3.6) depends only on the difference
r'-r, the function $\varphi$(r) has the same periodicity as q(r), and is,
therefore, the periodic cell flux. In the case where the cell
is symmetric, and the core center, r = O, coincides with the
center of a cell, $\varphi$(r) has the same phase as the source density
q(r); i.e., if q(r) is real, $\varphi$(r) is also real. This is the
case which is usually treated in the literature /3,4/. However,
the following equations hold also if the cell is asymmetric.

As is obvious from eqs. (3.5) and (3.6), the buckling method
has the advantage that a mathematically exact separation into
a macroscopic flux proportional to exp(i$\vec{B}\vec{r}$) and a microscopic
cell flux is possible. This advantage outweighs, to our opinion,
the principle problem of an "unphysical" extension of the equations
to regions where the flux is negative /5/. Clearly, the

resulting equations are valid only in the interior of
extended macroscopic regions of a reactor, which contain
a large number of cells. To examine the behaviour of neutron
flux and reaction rates near boundaries of macroscopic regions,
Böhme developed the code GITAN and used it to study several
important cases in slab geometry /8/.

These investigations showed that the separation method is
surprisingly good except in the immediate neighborhood of
region boundaries.
Recent attempts to develop an improved separation procedure
resulted in the more involved "asymptotic" method /5/, which
avoids the basic difficulty of the buckling method. However,
the procedure does not seem to lead to any more convincing re-
sults than the simple buckling method.

The simplest way to proceed further is to observe that the
balance equation (3.2) holds for the flux $\phi$ and the current
density J defined by eqs. (3.3) and (3.4). Integration over
an arbitrarily selected unit cell in the lattice gives

$$\int_{cell} d^3r \; \Sigma(r)\phi(r) + \int_{cell} d^3r \; div \, \vec{J}(r) = \int_{cell} d^3r \; Q(r) \tag{3.7}$$

The definition of the cell-averaged cross sections $\overline{\Sigma}_y$
(y is the reaction type) follows immediately from this balance
equation

$$\overline{\Sigma}_y = \frac{\int d^3r \; \Sigma_y \phi}{\int d^3r \; \phi} \tag{3.8}$$

The effective cell diffusion coefficient in the direction x is

$$\mathcal{D}_x = \frac{\int d^3r \; \partial J_x/\partial x}{B_x^2 \int d^3r \; \phi} \tag{3.9}$$

Similar equations hold for $D_y$ and $D_z$ .

These definitions are unique in the sense that they are in-
dependent of the choice of the cell. Therefore, it is easiest
to use the central cell. In principle, the cell-averaged
quantities could be evaluated from the definitions, using modern
computers. However, these equations are unnecessarily complicated
because they involve a dependence on the bucklings which is so
weak that there is no need to include it in practical calculations.
Therefore, one uses series expansions of $\phi(x)$ and $J(x)$ and
retains only the lowest order terms.

The expansion for $\phi$ is

$$\phi(r) = \left(\varphi_0 + i\,\vec{B}\,\vec{\varphi}_1 + \ldots\right)\left(1 + i\,(\vec{B}\vec{r}) + \ldots\right)$$

and for $J_x$

$$J_x = \left(j_{x0} - i\,(B_x\,j_{xx1} + B_y\,j_{xy1} + B_z\,j_{xz1}) + \ldots\right)\left(1 + i\,(\vec{B}\vec{r}) + \ldots\right)$$

It is possible to derive different approximations to the "exact"
definitions (3.8, 3.9) using these series expansions. The different
procedures, and the properties of the resulting definitions will
not be discussed in this report. The reader is referred to
/3,4,5/. Here it is simply stated that KAPER4 uses a $B^2$-inde-
pendent definition of the cross sections, i.e.

$$\Sigma = \frac{\int d^3r\,\Sigma\,\varphi_0}{\int d^3r\,\varphi_0} \qquad (3.10)$$

In evaluating the diffusion coefficient, one finds that the
first term, $j_{x0}$ does not contribute because of symmetry reason.
One obtains then, after some manipulations, which again will
not be repeated here

$$D_x = \frac{\int d^3r\,j_{xx1} + \int d^3r\,x\,\dfrac{\partial j_{xx1}}{\partial x}}{\int d^3r\,\varphi_0}$$

The second term in the numerator depends on the position
of the cell with reference to the "core center" r = 0,
because it contains the factor x. On the other hand, this
second term was shown to be small for fast reactor cases /3/,
and it is therefore neglected in KAPER4. Thus, the definition
used in KAPER4 is

$$\mathcal{D}_x = \frac{\int d^3r \, j_{xx1}}{\int d^3r \, \varphi_0} \tag{3.11}$$

This definition leads, after some additional manipulations,
/3,9/, to the well-known "Benoist formula" for a cell which is
composed of NR regions

$$\mathcal{D}_k = \frac{\sum_{i,j=1}^{NR} V_j \phi_j \, P_{ji,k} / \Sigma_i}{3 \sum_{j=1}^{NR} V_j \phi_j} \tag{3.12}$$

where k is the direction (parallel or perpendicular to the plates
or pins), and the $P_{jik}$ are the "directional" collision probabi-
lities which were first introduced by Benoist /10/.

These approximations, though rather low order, are accurate enough
for the usual fast-reactor cell calculations. One has, however,
to make sure that the balance equation is still fulfilled.
The above equation (3.7) can be written

$$\overline{\Sigma}\,\overline{\phi} + (\mathcal{D}_{\parallel} B_{\parallel}^2 + \mathcal{D}_{\perp} B_{\perp}^2)\overline{\phi} = Q \tag{3.13}$$

This equation is obviously fulfilled if the fluxes, as obtained
for the $B^2$-free case, are multiplied by the factor

$$\frac{\overline{\Sigma}}{\overline{\Sigma} + \sum_k \mathcal{D}_k B_k^2} \tag{3.14}$$

to account for the losses of neutrons due to leakage. In KAPER4
this is achieved by calculating the collision probabilities
for $B^2 = 0$, and then multiplying them by the above factor.
Thus, the spatial flux distribution is determined by the

zeroth-order flux $\phi_O$ and the correct flux normalization is
then obtained using the non-leakage factor (3.14).
It should be noted that the original definition (3.9) of
the diffusion coefficient accounts for the so-called "neutron
streaming" effect, the enhanced leakage out of a cell due to
non-uniform material distribution. Similarly, eq.(3.12) includes
the "streaming effect", at least in an approximate way. Note
that defining the transport-cross section as a simple flux-
volume-average over the cell is not consistent with the above
derivation. Eq.(3.12) is a good approximation if the cell con-
tains only materials with normal density. However, this equation
fails if the lattice contains voided (or nearly voided) regions
which extend in two dimensions.
In this case, the expansion in terms of the buckling does not
converge and the diffusion coefficient is infinitely large.
Then one has to use alternative methods, which are based on the
definition (3.9), but retain the buckling dependence. These methods
are not available in KAPER4; however, they are used in the stand-
alone programs PARDON /9/ for plate lattices, and ARIADNE for pin
lattices /5/.
For the computation in KAPER4, eq. (3.12) is written

$$D_k = \frac{\sum_j v_j \phi_j D_{jk}}{\sum_j v_j \phi_j} \tag{3.15}$$

where the "partial" diffusion coefficients $D_{jk}$ are

$$D_{jk} = \frac{1}{3} \sum_i P_{ji,k} / \Sigma_i \tag{3.16}$$

The latter quantities are computed in the collision probability
subroutines (ASLAB and BENOIS for plates, ACYL for pins) together
with the directional collision probabilities. However, since the
fluxes needed in eq. (3.15) are not known, the flux-volume averaging
is included in the outer iteration in the subroutine of the flux
equations (subroutine HETERO).

Note that the $D_{jk}$ are only auxiliary quantities for computation, which are not related to a "diffusion coefficient of region j". Regionwise diffusion coefficients are defined and used in the singularity option of KAPER4 (section 6.2).

## 3.2 Heterogeneous Flux and Adjoint Equations

To derive the multigroup equations for the cell flux, one has
to include the energy dependence in the integral equation
for the zeroth order flux

$$\Sigma_t(E,r)\,\varphi_0(E,r) = \int d^3r\,p(r',r;E)\,q(E,r') \qquad (3.17)$$

The source density $q(E,r)$ is composed of the fission source
and the slowing down source in the following manner

$$q(E,r) = \int dE'\left[\Sigma_\Delta(E'\to E,r)+\lambda\,\chi(E)\,\nu\Sigma_f(E',r)\right]\varphi_0(E',r) \qquad (3.18)$$

where $\lambda$ is the eigenvalue, $\chi(E)$ is the fission neutron spectrum.

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
q shows no resonance structure within this approximation. Then,
the straightforward procedure is to eliminate the source density q
between eqs.(3.17) and (3.18) and to write the multigroup equations
with the flux as a variable. If the unit cell is subdivided into
NR regions with index j, the resulting equations are

$$V_j\,\Sigma_{tj}^g\,\varphi_j^g = \sum_i P_{ij}^g \sum_k \left[\Sigma_{\Delta i}^{k\to g}+\lambda\chi^g\nu\Sigma_{fi}^k\right]V_i\,\varphi_i^k \qquad (3.19)$$

where $P_{ij}^g = <p_{ij}(E)>_g$, and the effective self-shielded cross
sections $\Sigma_{xj}^g$ are

$$\Sigma_{xj}^{g} = \frac{\sum_i \left\langle \frac{\Sigma_{xj}(E)}{\Sigma_{tj}} p_{ij}(E) \right\rangle_g V_i q_i^g}{\sum_i \left\langle \frac{1}{\Sigma_{tj}}(E) p_{ij}(E) \right\rangle_g V_i q_i^g} \qquad (3.20)$$

The brackets < > indicate averages over energy.

The method to calculate the effective cross sections will be described in Section 4.

The multigroup flux equations (3.19) are solved using 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. As mentioned earlier, leakage is included by scaling the collision probabilities in the following manner

$$P_{ij} \longrightarrow \frac{\overline{\Sigma}_t}{\overline{\Sigma}_t + \sum_k D_k B_k^2} P_{ij}$$

Since the fluxes needed to calculate the cell-averaged quantities $\overline{\Sigma}_t$ and $D_k$ (k = parallel or perpendicular to the plates or pins) are not known a priori, the calculation of the scaling factor is included in the outer iteration procedure in the solution of the flux equations.

KAPER4 also solves the equations adjoint to eq.(3.19), which read

$$\Sigma_{tj}^{g} \phi_j^{+g} = \sum_i \sum_k P_{ji}^k \left[ \Sigma_{ij}^{g \to k} + \lambda \chi^k \nu \Sigma_{fj}^g \right] \phi_i^{+k} \qquad (3.21)$$

The adjoint fluxes $\phi_j^{+g}$ are needed for the perturbation routine.

In KAPER4 eqs.(3.19) and (3.21) are used in a slightly more refined form for the fission source. The fission spectrum, $\chi^g$, 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 KAPER4-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 i as

$$\sum_m \chi_m^g \sum_k \nu \Sigma_{fmi}^k \, \nu_i^k \, \varphi_i^k$$

where m is the fissionable isotope index. This representation of the fission source is particularly important in the calculation of the reactivity worths (Section 6.1).

## 3.3  Remarks on the Output Quantities

As mentioned earlier, KAPER4 performs cell flux (or adjoint flux)
and eigenvalue calculations. The KAPER eigenvalues are useful
quantities to compare the reactivity of different cells, or to
compare eigenvalues of a heterogeneous and a homogeneous case.
However, the more commonly used output quantities are the cell-
averaged macroscopic group cross sections, which are stored in
the SIGMN block, and can be used in a subsequent whole-reactor
calculation, either in diffusion approximation, or by an $S_n$ code.
However, self-shielded KAPER cross sections, in the case of a
homogeneous composition are not equivalent to the results pro-
duced by the homogeneous cross-section processing program
GRUCAL, for two reasons:

- The method of calculating self-shielding in KAPER
  is not equivalent to the formulae used to interpolate
  f-factors in GRUCAL.

- The transport cross section produced by KAPER is ob-
  tained by combining the appropriate partial cross
  sections. These cross sections, as obtained e.g. from
  the KFKINR data set, are flux-weighted in energy and
  so are,then  also the KAPER transport cross sections.
  On the other hand, the transport cross sections usually
  taken from GRUCAL are current-weighted.
  Therefore, it has become customary to use the following
  procedure: First, homogeneous GRUCAL cross sections are
  produced, using smeared atom densities. Then, KAPER
  runs are carried out, both for the homogeneous case,
  and for the true heterogeneous cell. The difference
  of the two KAPER cross sections is then added to the
  GRUCAL SIGMN block. This way, it is assured that the
  "heterogeneous" and "homogeneous" cross sections are

comparable.

Alternatively, the GRUCAL SIGMN cross sections can be multiplied by the ratios of the heterogeneous and homogeneous KAPER cross sections. This method is prefered if either the heterogeneity correction is large, or if different number densities are used in KAPER4 and in GRUCAL. Further details are given in Section 6.3.2.

The SIGMN block contains transport cross sections rather than diffusion coefficients. KAPER produces either direction dependent or isotropic transport cross sections for the SIGMN block.

Note that the heterogeneous transport cross sections produced by KAPER4 are consistent with the effective cell diffusion coefficients defined in eq. (3.12). It is recommended to use the direction dependent transport cross sections, STR PA for parallel and STR PE for perpendicular (see Section 6.2) in whole-core diffusion calculations.
In $S_N$ calculations without explicit treatment of anisotropic scattering, either the isotropic transport cross sections, or the flux-volume averaged transport cross sections STR FV should be used instead of the total cross sections.

In addition, KAPER4 produces reaction rate distributions, and microscopic (regionwise or cell-averaged) reaction cross sections.

## 4. Resonance Self-Shielding

## 4.1 Rational Approximation of Reaction Coefficients

Fischer /1/ developed a method based on the theory of Wintzer /2/ for the determination of effective group cross sections for a reaction type x of an isotope $\nu$ in each region n of a unit cell. These cross sections are used in KAPER4 for the calculation of collision probabilities and the neutron balance as required in equation (3.19). For the determination of effective macroscopic cross sections a well defined prescription is given in equation (3.20). It was assumed without rigorous proof that these cross sections can be used for the calculation of average values of collision probabilities $P_{mn}$ as well.

The task then becomes to find a good approximation for reaction coefficients of isotope $\nu$ in energy group g defined by Wintzer /2/:

$$A_{x\nu mn} = \left\langle \frac{\sigma_{x\nu}(E)}{\sigma_{On} + \sigma_{t\nu}(E)} P_{mn}(\sigma_{t\nu}(E), \sigma_0) \right\rangle \qquad (4.1)$$

where $\sigma_{t\nu}(E)$ is the total cross section of the isotope $\nu$, $\sigma_{x\nu}(E)$ is the cross section of reaction type x of the isotope $\nu$ and $\sigma_{On}$ is the "background cross section" per atom of isotope $\nu$ due to the presence of other isotopes in cell region n. $A_{1\nu mn}$ is written for $A_{x\nu mn}$ calculated with $\sigma_{x\nu}(E) = 1$. The background cross section $\sigma_{On}$ is assumed to be constant in energy. The dependence of $p_{mn}$ on all background cross sections of the regions between m and n is indicated by the argument $\sigma_0$. Weighting with the number of atoms in the region volumes $V_m$ multiplied by the collision density $q_m$ and summation of (4.1) over all isotopes present in the unit cell yields the terms of the right hand side of (3.20).

For a homogeneous mixture the reaction coefficients $A_{x\nu mn}$ reduce to averages in energy, which can be directly looked up in the tables of self-shielding factors. Here, the right hand side of (4.1) has to be brought in a form suited for such a look-up as well. Therefore, Wintzer proposed to fit it to a series of partial fractions of the type:

$$\frac{p_{mn}(\sigma_{t\nu}(E), \sigma_0)}{\sigma_{t\nu}(E) + \sigma_{0n}} \simeq \sum_{i=1}^{NB} \frac{a_i}{b_i + \sigma_{t\nu}(E)} \tag{4.2}$$

If this fit is used in (4.1), the averaging over energy becomes

$$\left\langle \frac{\sigma_{x\nu}(E)}{b_i + \sigma_{t\nu}(E)} \right\rangle = \frac{\langle \sigma_{x\nu}(E) \rangle \, f_x(b_i)}{b_i + \langle \sigma_{t\nu}(E) \rangle \, f_t(b_i)} \tag{4.3}$$

where $\langle \sigma_{x\nu}(E) \rangle$ are cross section averages at infinite dilution and $f_x(b_i)$ are tabulated self-shielding factors defined as

$$f_x(\sigma_0) \, \langle \sigma_{x\nu}(E) \rangle = \left\langle \frac{\sigma_{x\nu}(E)}{\sigma_{t\nu}(E) + \sigma_0} \right\rangle \Big/ \left\langle \frac{1}{\sigma_{t\nu}(E) + \sigma_0} \right\rangle \tag{4.4}$$

The collision density $q_m$ can - in principle - be calculated iteratively, starting with an estimate calculated using fully shielded total cross sections and a flat flux distribution in the whole cell. Experience has shown that the iteration procedure on the collision density does not change calculated effective cross sections significantly under this condition. It is therefore omitted in KAPER.

Effective microscopic cross sections of reaction type x of isotope $\nu$ in region n, $\sigma_{x\nu n}$, which are fairly independent of the fit (4.2), can now be calculated as the ratio

$$\sigma_{x\nu n} = \frac{\sum_m A_{x\nu mn} V_m q_m}{\sum_m A_{1\nu mn} V_m q_m} \tag{4.5}$$

## 4.2 On the Choice of Parameters in the Rational Approximation

The accuracy of the fit (4.2)

$$\frac{P_{mn}(\sigma_{t\nu}, \sigma_0)}{\sigma_{t\nu} + \sigma_{0n}} \simeq \sum_{i=1}^{NB} \frac{a_i}{b_i + \sigma_{t\nu}}$$

depends somewhat on the choice of the mesh points $b_i$. An approximation fairly independent of the parameters chosen can be achieved by use of recommended parameters:

NB should be between 4 and 10, default is NB = 6.

$b_1$ should be of the magnitude of the fully shielded total cross section, $\sigma_{t\nu} \times f_t(\sigma_0 = 0)$. In KAPER4 it is set to the minimum min $(\sigma_{t\nu} \times f_t(\sigma_0 = 0), \sigma_{0n})$, where n = 1,NR. If this value is < 1 barn the lowest value $b_1$ is chosen to be 1 barn. The maximum test cross section $b_{NB}$ is set to GAM×$b_1$. It is recommended to set GAM = 1000. For isotopes with very pronounced resonance peaks a higher value of GAM may be more appropriate. The intermediate cross sections $b_i$ are equally spaced between the extrema on a log-scale.

With the recommended choice it may happen that calculated effective cross sections in regions with high $\sigma_0$ (e.g. regions containing highly diluted isotopes) become larger than the cross section calculated for this dilution $\sigma(\sigma_{0n})$ or even $\sigma(\sigma_0 = \infty)$. In these cases the effective cross section in region n is set equal to the cross section calculated for $\sigma_{0n}$, i.e. about the infinite dilution cross section. A warning is printed, if this enforced correction exceeds 1%.

By increasing NB and GAM the number of warnings can be reduced for certain resonances, but usually the final result is not altered. A general remedy which prevents this inaccuracy cannot be given.

An example showing the influence of a variation of parameters is given in Tab. 8.3.

The quantity EPS can be used to modify the approximation (4.2) by subtracting $EPS \times p_{mn}(b_1, \sigma_0)$ from $p_{mn}(\sigma_{t\nu}, \sigma_0)$ on the left hand side prior to the approximation. $p_{mn}(b_1, \sigma_0)$ is a collision probability calculated using $b_1$ as a constant test cross section for isotope $\nu$. This ensured the smooth transition to the homogeneous case for decreasing optical thicknesses in former versions of KAPER. For KAPER4 this whole part of the program has been newly coded. The transition to the homogeneous case requires no particular provisions anymore, as is demonstrated in the example given in Tab. 8.1. Thus, EPS = 0. can be set without significantly influencing the results.

Another modification of the program can be achieved by setting EPS < 0. In this case the background cross section $\sigma_0$ for isotopes is calculated using the potential cross section of the isotope $^{238}U$ and unshielded total cross sections for all other isotopes (TYPE STOTW), as it is done in the cross section preparation code GRUCAL /22/ for homogeneous mixtures. However, the standard procedure in KAPER4 with EPS.GE.0. is the use of the effective total cross section of $^{238}U$ and of unshielded total cross sections of all other isotopes for the calculation of $\sigma_0$. Results of both options can be found in Tab. 8.3, too.

## 5. Calculation of Collision Probabilities and Cell Diffusion Coefficients

### 5.1 Collision Probabilities for Slab Lattices

The calculation of collision probabilities is still performed as described in former reports /1/:

In a lattice made up of slab cells periodic boundary conditions are assumed in the direction perpendicular to the plates. Reflective boundary conditions have to be simulated by doubling the number of regions. Infinite extension of the plates is assumed in two orthogonal directions (see Fig. 7.1).

The optical thickness $x_n$ of a slab n of geometrical thickness $t_n$ and total macroscopic cross section $SIGT_n$ is defined as:

$$x_n = SIGT_n \times t_n.$$

The optical thickness of all regions j between slabs m and n is

$$x_T = \sum_{\substack{j<n \\ j>m}} x_j.$$

With the assumption of a flat flux distribution in regions m and n the first flight collision probability of neutrons born in m and colliding in n, $P_{mn}$, becomes:

$$P_{mn} = \frac{1}{2x_n} \{ E_3(x_T) - E_3(x_T+x_m) - E_3(x_T+x_n) + E_3(x_T+x_m+x_n) \} \tag{5.1}$$

and

$$P_{nn} = 1 - x_n^{-1} \{ E_3(0) - E_3(x_n) \} \tag{5.2}$$

$E_k$ is the exponential integral of order k, defined as

$$E_k(x) = \int_0^1 t^{k-2} \exp(-x/t) \, dt \qquad \text{for } k \geq 1$$

and $E_k(0) = (k-1)^{-1}$ for k>1.

In KAPER4 exponential integrals are calculated from the function $E_1(x) = -Ei(-x)$ (supplied by the library function MMDEI of IMSL /11/) using the recursion formula

$$(k-1) \, E_k(x) = \exp(-x) - x \, E_{k-1}(x) \qquad \text{for } k>1.$$

For infinite lattices of optical cell width $x_c$ the summation over all targets n is carried out by the quadrature method proposed by Olson /12/:

$$\sum_{n=0}^{n=\infty} E_k(x + x_c n) \simeq \sum_{i=1}^{i=4} w_{ki} \exp(-x x_{ki})$$

$w_{ki}$ and $x_{ki}$ are tabulated in KAPER4. The error of this formula is claimed to be $\leq 10^{-5}$.

For the calculation of directional collision probabilities for direction $\kappa$, $P_{mn\kappa}$ - as required for Benoist's diffusion coefficient eq. (3.12) - the function $E_3$ in eqs. (5.1) and (5.2) is replaced by $3 \times E_5$ for the direction normal to the slabs and by the function $3/2(E_3 - E_5)$ for the direction parallel to the slabs.

Again, Olson's formulas are used for the summation of $P_{mn\kappa}$ over all cells of an infinite lattice.

The accuracy of each term in (5.1) is about $1 \times 10^{-5}$ using single precision in (5.1) and double precision for the calculation of the functions $E_k$. Experience has shown that this precision is sufficient for most cell calculations in slab geometry. In cases of very thin regions $P_{mn}$ can be calculated using an approximation of Wintzer /2/ for $E_3$:

$$E_3(x) \simeq \sum_{i=1}^{i=7} a_i \exp(-b_i x)$$

$a_i$ and $b_i$ are tabulated in KAPER, too. The error of this approximation is said to be of the order $< 10^{-3}$ for $0.002 < x < 2$. Using this approximation the summation of (5.1) over all cells of an infinite lattice becomes possible in closed form. The reciprocity relation is maintained and the transition to infinitely thin regions is exact. This may improve the results slightly, as is demonstrated in the example given in Tab. 8.1, case NHOM=1.

The approximation of Wintzer is always used for the calculation of $p_{mn}$ of eq. (4.2) in slab geometry needed in the cross section preparation phase (see chapt. 3.1).

## 5.2 Cylindrical Geometry (Subroutine ACYL)

The subroutine ACYL calculates isotropic and/or directional collision probabilities in cylindrical geometry, i.e. for pin lattices, or for singularities. The collision probabilities are in turn used to calculate the cell fluxes (and adjoint fluxes), and also the (isotropic or directional) cell diffusion coefficients. Note that the cross-section preparation part in KAPER4 uses a different collision probability routine, PMNBIC, which is simpler because it calculates only isotropic collision probabilities. However, the same methods are used in both routines. Therefore, it is sufficient to develop only the equations for ACYL in this section.

### 5.2.1 Capabilities of ACYL

The pin lattice geometry is more complicated than the plane case because it is twodimensional. ACYL calculates collision probabilities using either of the following two approximations:

- cylindricalize the cell, and assume that neutrons leaving the cell enter the next one, with an isotropic angular distribution ("white boundary condition"). The actual problem is thus reduced to an artificial one-dimensional problem.
  Note that there is no difference between a square and a hexagonal lattice, in this approximation.

- to improve on the "white" boundary condition at an imaginary cell boundary, the collision probabilities in the irregularly shaped coolant channel (the "Dancoff factor") can be calculated by an approximate method (the so-called "Sauer-method").

ACYL performs the following calculations:

- The in-cell collision probability $P_{ij}^*$ (probability that a neutron born in region i collides in region j of the same cell); both isotropic and directional $P_{ij}^*$ can be calculated. The numerical method developed by Carlvik / 14/ and by Kavenoky /15 / is used.

- The lattice collision probability $P_{ij}$ (probability that a neutron born in region i collides in region j of any cell in the lattice).
In the cylindrical cell approximation, this probability is given by the equation

$$P_{ij} = P_{ij}^* + P_{ib}^* P_{bj}^* \left[ 1 + \sum_{h=1}^{\infty} (P_{bb}^*)^h \right] \qquad (5.3)$$

where $P_{ib}^*$ is the probability that a neutron escapes from the cell where it was born; $P_{bb}^*$ is the probability that a neutron entering the cell traverses it without a collision. The equation for $P_{ij}$ can be written

$$P_{ij} = P_{ij}^* + \frac{V_j \Sigma_j P_{ib}^* P_{jb}^*}{\sum_h V_k \Sigma_k P_{kb}^*} \qquad (5.4)$$

where $V_i$ is the volume, $\Sigma_i$ the total (or transport) cross section of the region i. The escape probability $P_{ib}^*$ is given by (NR number of regions)

$$P_{ib}^* = 1 - \sum_{j=1}^{NR} P_{ij}^*$$

Note that eq.(5.4) also holds for directional collision probabilities. However, the flux impinging on the cell boundary from outside is then assumed to have an angular distribution proportional to $\Omega_k^2$, where $\Omega_k$ is the cos between the neutron flight path, and the direction k (parallel or perpendicular to the axis).


- The (isotropic or directional) "partial" cell diffusion coefficients, defined by eq.(3.16) in Section 3.1, are also calculated. However, the flux volume averaging required to obtain the diffusion coefficient

$$\mathcal{D}_k = \frac{\sum_i \mathcal{V}_i \phi_i \mathcal{D}_{ik}}{\sum_i \mathcal{V}_i \phi_i} \qquad (5.5)$$

is performed in the routine HETERO.

- As an option, ACYL calculates Dancoff factors for the outer-most region of a cell (coolant channel). The method by Sauer /16/ is used for the isotropic case. The anisotropic Dancoff factor can be written as an integral. In ACYL, an approximation to this integral is used which is valid for small optical thicknesses (i.e. for most fast reactor cells).

## 5.2.2   Calculation of the In-Cell Collision Probabilities

Carlvik /14/ and Kavenoky   /15 / showed that the $P_{ij}^*$, which are originally defined by a 6-fold integral, can be reduced to a single integration over Bickley functions

$$P_{ij}^* = \frac{2}{\mathcal{V}_i} \int_0^{R_i} f(h)\,dh \qquad (5.6)$$

where

$$f(h) = \frac{1}{\Sigma_i} \left\{ Ki_3 (t_{j-1}+t_{i-1}) - Ki_3 (t_{j-1}+t_i) - Ki_3(t_j+t_{i-1}) \right.$$

$$\left. + Ki_3(t_j+t_i) - Ki_3|t_{j-1}-t_{i-1}| + Ki_3|t_{j-1}-t_i| + Ki_3|t_j-t_{i-1}| - Ki_3|t_j-t_i| \right\} \qquad (5.7)$$

where $Ki_3$ is the Bickley function of index 3, and the $t_i$ etc. are distances, measured in free paths(see Figure 1). The diagonal term is given by

$$P_{ii}^* = 1 + \frac{2}{\mathcal{V}_i} \int_0^{R_i} g(h)\,dh \qquad (5.8)$$

where

$$g(h) = \frac{1}{\Sigma_i} \left\{ Ki_3(2t_{i-1}) + Ki_3(2t_i) - 2Ki_3(t_i + t_{i-1}) \right.$$

$$\left. + 2Ki_3(t_i - t_{i-1}) - 2Ki_3(0) \right\} \tag{5.9}$$

The numerical integration from O to $R_i$ is carried out by Gauss quadrature, using 2 times 3 mesh points in each range $R_{k-1}$ to $R_k$ (k <i). The Ki-functions are computed by subroutine functions, which use the Chebysheff approximations obtained by Gargantini and Pomentale /17/. The accuracy is $0.3 \times 10^{-7}$ or better.

This procedure is used directly for the "general" case, eqs. (5.6, 5.7). Special cases will be discussed now.

## Diagonal element, $\Sigma_i$ > O

For the pin cells of a fast reactor, $P_{ii}^*$ may be as low as $10^{-2} - 10^{-3}$. Thus, the integral in eq. (5.8) is negative, and compensates most of the first term, so that the accuracy becomes poor. It was found that better results are obtained if the "One" in eq. (5.8) is represented as an integral

$$1 = \frac{4}{V_i} \int_0^{R_i} (y_i - y_{i-1}) \, dh \tag{5.10}$$

where $y_i^2 = R_i^2 - h^2$.
In ACYL, the term (5.10) is combined with the second (integral) term in eq. (5.8).

Optically thin region, $\Sigma_j \sim 0$ (e.g. voided channel)

In KAPER4, macroscopic cross-sections are not allowed to be zero. Therefore, the distinction of a number of different cases, which was worked out by Kavenoky for zero cross-sections, is not necessary. To keep the routine ACYL simple, the following approach to handle small cross-sections was adopted.

First, it was found that for cross-sections $> 2 \times 10^{-4} cm^{-1}$, eqs. (5.6) and (5.7) give sufficient accuracy. To improve the accuracy somewhat, and to make use of the rather good approximation in the Ki-function routines, eq. (5.7) is evaluated with double precision in ACYL. The user should, however, make sure that a small amount of material ($\Sigma \geq 2 \times 10^{-4}$) is smeared in the voided region.

The accuracy for the diagonal element, eqs. (5.8 - 5.10), is, however, worse. Therefore, the expression (5.8) is split in two terms. The first term

$$P_{ii}^{*(1)} = \frac{2}{V_i} \int_0^{R_{i-1}} dh \left\{ 2(y_i - y_{i-1}) + \frac{1}{\Sigma_i} \left( Ki_3(2t_{i-1}) + Ki_3(2t_i) - 2Ki_3(t_i + t_{i-1}) \right) \right\} \quad (5.11)$$

refers to the neutrons which go through inner regions (assume $i \geq 2$). It is calculated numerically, like the off-diagonal elements.

The second term refers to neutrons which collide in region i without leaving it. It can be written as

$$P_{ii}^{*(2)} = \frac{2\Sigma_i}{V_i} \int_0^{R_{i-1}} dh \, (y_i - y_{i-1})^2 Ki_1'(0)$$

$$+ \frac{4\Sigma_i}{V_i} \int_{R_{i-1}}^{R_i} dh \, y_i^2 Ki_1'(0) \quad (5.12)$$

It can be shown that eq. (5.12) is equivalent to

$$P_{ii}^{*(2)} = \frac{1}{2} \bar{\ell} \sum_i \overline{(\ell/\bar{\ell})^2}$$

where $\ell$ is the chord length in region i. For an infinite hollow cylinder, the second moment is given by

$$F = \overline{\left(\frac{\ell}{\bar{\ell}}\right)^2} = \frac{4 - 3k(1-k^2) - 2(1+k^2)E(k^2) + 2(1-k^2)K(k^2)}{3(1-k^2)(1-k)} \qquad (5.13)$$

where $k = R_{i-1}/R_i$, and E and K are the complete elliptic integrals of the first and second kind /18/. In ACYL, the function (5.13) is approximated as follows:

For k < 0.7 by the series expansion

$$F = \frac{4\left[1 - 0.75k - 1.1781k^2 + 0.75k^3 + 0.1473k^4 + 0.0184k^6\right]}{3(1-k^2)(1-k)} \qquad (5.14)$$

For k > 0.8 by the asymptotic expression

$$F = 0.875 + 0.25 \ln\frac{16}{1-k^2} - \frac{1-k^2}{12} \qquad (5.15)$$

For k between 0.7 and 0.8, a linear interpolation between eqs. (5.14) and (5.15) is used.

These equations for $P_{ii}^{*}$ are used if the optical thickness of region i is less than 0.001.

## Thin Cells

To make sure that reasonable results are obtained if KAPER4
is used in the "quasi-homogeneous" limit, i.e. very thin cells,
the following approximations are used if the cell radius is less
than 0.04 cm:

Diagonal elements:

$$P_{ii}^{*} = \frac{1}{2} \bar{\ell}_i \Sigma_i \left[ F(k) + F_2(k) D_{i-1} \right] \qquad (5.16)$$

In this equation, $F_2$ is the first integral in eq. (5.12); it
is given by

$$F_2 = F - \frac{2(2+k)}{3(1+k)} \qquad (5.17)$$

and $D_{i-1}$ is the transmission probability through the inner
regions (<i), which is represented in the limit of thin cells as
a product of Wigner rational approximations for each region

$$D_{i-1} = \widetilde{\prod_{j<i}} \frac{1}{1 + \bar{\ell}_j \Sigma_j} \qquad (5.18)$$

The off-diagonal elements (j>i) are approximated by

$$P_{ij}^{*} = \left( 1 - P_{ii}^{*} - \sum_{k<i} P_{ik}^{*} \right) \frac{\bar{\ell}_j \Sigma_j}{1 + \bar{\ell}_j \Sigma_j} \widetilde{\prod_{i<k<j}} \frac{1}{1 + \bar{\ell}_k \Sigma_k} \qquad (5.19)$$

Directional Collision Probabilities

As far as integrals over Ki-functions are involved , it is easy
to derive the directional collision probabilities. One has to
replace

$$\text{for } P_{\perp} : \text{Ki}_n \text{ by } \frac{3}{2}\text{Ki}_{n+2}$$

$$\text{for } P_{//} : \text{Ki}_n \text{ by } 3(\text{Ki}_n - \text{Ki}_{n+2})$$

For an optically thin region, one has to multiply $P_{ii}^{*(2)}$, which
is defined by eq.(5.12), by the "anisotropy factor" (0.75 for
perpendicular, 1.5 for parallel). For thin cells, all the $P_{ij}^{*}$
are multiplied by these factors.

## 5.2.3  Lattice Collision Probabilities, Cell Diffusion Constants

The evaluation of the eqs. (5.3 - 5.5) is straightforward, once
the in-cell collision probabilities are available. One comment
should be made:
The physical relation

$$D_{iso} = \frac{1}{3} D_{//} + \frac{2}{3} D_{\perp} \tag{5.20}$$

is no longer exactly satisfied if the cylindrical-cell approximation
(5.3) is used.

## 5.2.4  Use of the Dancoff Factor

In a hexagonal or square lattice, the coolant channel has an
irregular shape, and the approximation as a cylindrical shell is
artificial, especially if the channel is voided. Alternatively,
one can use the Dancoff factor $\Gamma$, which is defined as the pro-
bability that a neutron entering the coolant channel makes a
collision without re-entering a fuel rod.

Exact calculations of the Dancoff-factor are possible, but
rather cumbersome. In ACYL, a fairly simple but rather accurate
approximation, suggested by Sauer and described in detail in
Ref. /16/, is used.

In this case, the equations (5.6) etc. are used only for a
"reduced cell", which consists of the regions 1 to NR-1. The Dancoff
factor is defined for region NR(the coolant channel). If $P^*_{ib}$ is
now the probability that a neutron born in i escapes from the
reduced cell, the equation for the lattice collision probabili-
ties is (i,j $\leq$ NR-1)

$$P_{ij} = P^*_{ij} + \frac{P_{ib}(1-\Gamma)\, 4\, V_j\, \Sigma_j\, P^*_{jb}}{S_b\, \Gamma + (1-\Gamma) \sum_k 4\, V_k\, \Sigma_k\, P^*_{kb}} \tag{5.21}$$

where $S_b$ is the surface (per unit height) of the reduced cell.

The problem of calculating a directional Dancoff factor, $\Gamma_\perp$ or
$\Gamma_{\parallel}$, is more involved.
The appropriate definition is given as the collision probability
for neutrons entering the surface with an angular distribution
~ $\Omega^2_k$, where

$$\Omega^2_k = \begin{cases} \cos^2\vartheta & k = \parallel \\ \frac{1}{2}\sin^2\vartheta & k = \perp \end{cases}$$

$\Omega_k$ is the angle between the axis and the direction of the incoming
neutron. The definition is then

$$\Gamma_k = \frac{\int dS \int d\Omega\,(n\Omega)\,(1 - e^{-\ell(S,\Omega)\Sigma})\,\Omega^2_k}{\int dS \int d\Omega\,(n\Omega)\,\Omega^2_k} \tag{5.22}$$

S is the surface, (n$\Omega$) the cos between the surface normal and the
incoming neutron.

To calculate $\Gamma_k$ in a manner similar to Sauer's method, one notes that the latter is based on approximating the chord length distribution function, $f(\ell)$, by a decaying exponential function, shifted by a length $t = \tau\bar{\ell}$ . To calculate $\Gamma_k$, it is more appropriate to assume an approximation for the distribution $g(\rho)$, where $\rho$ is the projection of the chord length on the plane perpendicular to the pins. The $\Gamma_k$ can then be written

$$\Gamma_{\perp} = 1 - \frac{16}{3\pi} \int_0^{\infty} d\rho \, g(\rho) \, Ki_5(\Sigma\rho)$$

$$\Gamma_{\parallel} = 1 - \frac{16}{\pi} \int_0^{\infty} d\rho \, g(\rho) \left[ Ki_3(\Sigma\rho) - Ki_5(\Sigma\rho) \right] \qquad (5.23)$$

$$\Gamma_{iso} = 1 - \frac{4}{\pi} \int_0^{\infty} d\rho \, g(\rho) \, Ki_3(\Sigma\rho)$$

It follows from these equations (and of course also from the definition (5.2.2)) that the relation

$$\Gamma_{iso} = \frac{1}{3} \Gamma_{\parallel} + \frac{2}{3} \Gamma_{\perp}$$

does not hold. One expects, therefore, that the corresponding relations between the $P_{ijk}$, which hold if the $P_{ijk}$ are calculated exactly, are not preserved in the present approximation.

It is easily seen that the integrals (5.23) cannot be evaluated analytically, if $g(\rho)$ is approximated by a decaying exponential function. However, coolant channels in fast reactors are usually optically thin. Therefore, an expansion for small $\bar{\ell}\Sigma$ is of interest

$$\Gamma_\perp = \frac{8}{9} \bar{\ell} \Sigma - \frac{1}{3} \bar{\ell^2} \Sigma^2$$

$$= \frac{8}{9} \bar{\ell} \Sigma \left(1 - \frac{3}{8} \bar{\ell} \Sigma F\right)$$

$$\Gamma_\parallel = \frac{4}{3} \bar{\ell} \Sigma - \bar{\ell^2} \Sigma^2 \qquad\qquad (5.24)$$

$$= \frac{4}{3} \bar{\ell} \Sigma \left(1 - \frac{3}{4} \bar{\ell} \Sigma F\right)$$

Using Sauer's approximation, the factor F is given by

$$F = 1 - \tau + \frac{\tau^2}{2}$$

where $\tau$ is the "geometric index" defined by Sauer /16/.

The expressions (5.24) are accurate enough for the sodium channels in a fast reactor (and, of course, for voided channels). However, to make sure that no negative values can be produced, the following equation is used in ACYL for the difference $\Delta\Gamma_k$

$$\Delta\Gamma_k = \Gamma_k - \Gamma_{iso} \approx \left(\frac{1}{\zeta_k} - 1\right) \bar{\ell} \Sigma \exp\left(-\frac{3}{2} F \bar{\ell} \Sigma\right) \qquad (5.25)$$

where
$$\zeta_k = \begin{cases} 9/8 & k = \perp \\ 4/3 & k = \parallel \end{cases}$$

The series expansion of (5.25) is consistent with the equations (5.24).

## 5.2.5  Results for Anisotropic Cell Diffusion Coefficients

Calculations of the isotropic and directional diffusion coeffi-
cients were carried out for the cell of a gas cooled fast breeder
reactor, using a two-region calculation. The cell geometry is
determined by the pin radius, a = 0.37 cm, and the pitch of the
(hexagonal) lattice, s = 1.08 cm. The equivalent radius of the
cell is $R_2$ = 0.56702 cm. Both the cylindrical cell model (with
white boundary conditions), and the Dancoff factor method were
used.
Table 5.1 shows the results for a voided cell, with a fictitious
low cross-section, 0.0002 $cm^{-1}$, of the coolant channel. The
cross-section of the pin was varied from 0.1 to 1.0 $cm^{-1}$.

-   While the isotropic diffusion coefficients obtained with
    the two methods are fairly well consistent, considerable
    differences exist between the directional diffusion coefficients.
    In each case, $\Delta D_r$ is smaller, and $\Delta D_z$ larger with the Dancoff
    method, than with the cylindrical cell method.

-   These differences reflect the errors in the cell method, where
    a given angular distribution is assumed for neutrons entering
    a cell, or the fuel region. This assumption, apparently, is
    not well justified for the directional collision probabilities.

-   The physical relation

$$D_{iso} = \frac{1}{3} D_{\parallel} + \frac{2}{3} D_{\perp}$$

    is not fulfilled for the Dancoff method. The reason, obviously,
    is again that the assumed angular distribution is not correct.

- Nevertheless, the cell model provides a simple method to obtain an estimate for the anisotropic diffusion coefficients in voided lattices. For more accurate calculations (which are beyond the scope of the code KAPER4), more involved methods should be used. Note that a routine which uses a $B^2$-dependent method for an infinite lattice (ARIADNE) is available at KfK /5/.

Table 5.2 shows the results for variable coolant cross-sections, $\Sigma_2$, assuming that $\Sigma_1$ is constant. It is interesting to note that the ratio $\Delta D_z / \Delta D_r$ seems to have a characteristic value for each of the two methods; this value changes rather little as the coolant cross-section increases, and the heterogeneity effect becomes smaller.

6.        Special Options of the Code

6.1      Perturbation Option in Slab Geometry

6.1.1    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 dis-
turbed. We shall call this cell containing the local perturbation,
including the surrounding unit cells in which the flux is signi-
ficantly 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 KAPER4 program, for the slab geometry
case.

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 ob-
tained by solving the integral transport equation, eq. (3.19), 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. (3.19) 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 imagi-
nary 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:

$$v_j \Sigma_j^g \phi_j^g = \sum_i P_{ij}^{+g} \sum_k \left[ \Sigma_{si}^{k \to g} + \chi^g \nu \Sigma_{fi}^k \right] v_i \phi_i^k + q_j^g \qquad (6.1)$$

where $P_{ij}^+$ is the probability that a neutron from region i suffers its
first collision in region j while remaining within our imaginary
boundaries. The fluxes and cross sections explicitly written in
eq. (6.1) are defined for the regions that compose the perturbed
cell. Therefore the first term on the right-hand side of eq.(6.1)
represents the contributions from within our imaginary boundaries
and the second term ($q_j^g$) the contribution from outside the boun-
daries. The source term $q_j^g$ has an appearance similar to the first
term in eq.(6.1) except that the collision probabilities have a
different definition. We may write the source equation as

$$q_j^g = \sum_i \varepsilon_{ij}^g \sum_k \left[ \Sigma_{si}^{k \to g} + \lambda \chi^g \nu \Sigma_{fi}^k \right] v_i \phi_i^k \qquad (6.2)$$

where $\varepsilon_{ij}$ is the probability that a neutron in a region i outside
our imaginary boundaries suffers its first collision in a region
j inside the boundaries. The cross sections and fluxes in eq.(6.2)
are defined for the normal unit cell and are available from a
previous calculation. Therefore $q_j^g$ can be calculated directly
and used in eq.(6.1) to solve for the flux within the perturbed
cell (inside the imaginary boundaries).

The solution of both eq.(6.1) and the corresponding adjoint
equation are carried out by the power iteration method as
briefly outlined in Section 3.2.

## 6.1.2  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 KAPER4 program rather than a first-order form
as is commonly employed in perturbation programs. Therefore
formulating the perturbation equation with the integral trans-
port theory flux equation (representing the perturbed state) and
the adjoint equation (representing the unperturbed state) one
obtains

$$\rho = \frac{1}{\mathcal{D}_{\rho}} \sum_{g} \sum_{i} v_{i} \phi_{i}'^{g} \left[ -\delta \Sigma_{ti}^{g} \phi_{i}^{+g} + \sum_{j} \sum_{k} \delta(\Sigma_{si}^{g \to k} P_{ij}^{k}) \phi_{j}^{+k} \right.$$

$$\left. + \lambda \sum_{n} \sum_{k} \sum_{j} \delta(\chi_{n}^{k} v \Sigma_{fin}^{g} P_{ij}^{k}) \phi_{j}^{+k} \right] \qquad (6.3)$$

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 $\delta N$, 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 n) from each fissionable isotope present. The denominator of eq.(6.3) is

$$\mathcal{D}_{\rho} = \lambda' \sum_{g} \sum_{i} v_{i} \phi_{i}'^{g} \sum_{n} v \Sigma_{fin}'^{g} \sum_{k} \sum_{j} \chi_{n}'^{k} \phi_{j}^{+k} P_{ij}'^{k} \qquad (6.4)$$

We may rewrite eq.(6.3) if we use the following form of the perturbation operator:

$$\delta(\Sigma_{i} P_{ij}) = (\delta\Sigma_{i}) P_{ij} + \Sigma_{i}'(\delta P_{ij})$$

In addition, we may also use the relationship between the source importance function $\psi_{i}^{+k}$ and the colliding neutron importance function $\phi_{j}^{+k}$

$$\psi_{i}^{+k} = \sum_{j} P_{ij}^{k} \phi_{j}^{+k}$$

Introducing these relationships into eq.(6.3) we can write the results as, after some rearranging,

$$S = \frac{1}{D_\varsigma} \sum_g \sum_i \mathcal{V}_i \phi_i'^g \left[ -\delta \Sigma_{ai}^g \phi_i^{+g} + \sum_k \delta \Sigma_{\delta i}^{g \to k} (\psi_i^{+k} - \phi_i^{+g}) \right.$$

$$\left. + \lambda \sum_n \sum_k \delta (\chi_n^k \nu \Sigma_{fin}^g) \psi_i^{+k} + \sum_k \sum_j (\Sigma_{\delta i}'^{g \to k} + \lambda \sum_n \chi_n'^k \nu \Sigma_{fin}'^g) \delta P_{ij}^k \phi_j^{+k} \right] \tag{6.5}$$

where $\Sigma_{ai}^g$ is the total absorption cross section in region i
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. (6.5) accounts for diffusion
effects.

The form utilized in the KAPER4 program is, however, slightly
different than eq. (6.5). We can rearrange the equation to obtain
the following results

$$S = \frac{1}{D_\varsigma} \sum_g \sum_i \mathcal{V}_i \phi_i'^g \left[ -\delta \Sigma_{ai}^g \psi_i^{+g} + \sum_k \delta \Sigma_{\delta i}^{g \to k} (\psi_i^{+k} - \psi_i^{+g}) \right.$$

$$+ \lambda \sum_n \sum_k \delta (\chi_n^k \nu \Sigma_{fin}^g) \psi_i^{+k} + \delta \Sigma_{ti}^g (\psi_i^{+g} - \phi_i^{+g}) \tag{6.6}$$

$$\left. + \sum_k \sum_j (\Sigma_{\delta i}'^{g \to k} + \lambda \sum_n \chi_n'^k \nu \Sigma_{fin}'^g) \delta P_{ij}^k \phi_j^{+k} \right]$$

The only advantage of eq. (6.6) is that the first three terms
can be identified as the normal absorption, scattering, and
fission perturbation terms.

The perturbed flux in eq. (6.6) is obtained with the procedure
explained earlier in this Section. In this case the disturbance
in the unit cell is the inserted reactivity sample. By utilizing
eq.(6.1) 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 KAPER4-program is a lattice program the denominator
of eq.(6.6) can not be calculated for the entire assembly core
and reflector. The calculation of the denominator, or normali-
zation 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

$$D_\varrho = F(0) D_{NOR}$$

where

$$D_{NOR} = \frac{\lambda \sum_g \sum_i v_i \phi_i^g \sum_n v \Sigma_{fin}^g \sum_k \sum_j \chi_n^k \phi_j^{+k} P_{ij}^k}{\sum_j v_j}$$

and

$$F(0) = \frac{\int d^3 r \sum\limits_{n} \sum\limits_{g} \nu \Sigma_{fn}^g (r) \phi^g(r) \sum\limits_{k} \chi_n^k \psi^{+k}(r)}{\sum\limits_{n} \sum\limits_{g} \nu \Sigma_{fn}^g \phi^g(0) \sum\limits_{k} \chi_n^k \psi^{+k}(0)}$$

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 approximation 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 whole-core two-dimensional diffusion calculation, and is used as input data to KAPER4.

## 6.2  Option for the Diffusion Coefficient of a Singularity

The singularity option is designed to obtain cross sections and diffusion coefficients which are averaged over a core singularity, e.g. control rod followers (with or without sodium) or absorber rods.
For the KAPER4 calculations, the singularity must be cylindricalized, and surrounded by a homogeneous region of core material (region NR).The reaction cross sections are then simply flux-volume-averaged over the (NR-1) regions of the singularity.

The only quantity which is treated in a different way than in standard KAPER4 is the diffusion coefficient. It is known that

diffusion theory greatly overestimates the leakage in low-density regions of a core if the diffusion coefficient is defined as $1/(3\Sigma tr)$ /9, 19/. Therefore, an alternative definition of the diffusion coefficient is used in this option, which remains valid if the material density in the singularity is very low (e.g. voided control rod follower).

This definition was proposed by Rowlands and Eaton /19/. For the use in KAPER4, it was extended to a multiregion configuration.

The equations for the diffusion coefficient of the singularity are derived in the following section. Then, the validity of the flux-volume averaging procedure for the homogenization of absorber rods is discussed. In a further section, comments on the use of this option for low-density singularities, and for absorber rods are summarized.

## Calculation of the Effective Diffusion Coefficient for a Singularity

When defining an axial diffusion coefficient for a core singularity, one should make sure that the definition remains valid for low-density regions, e.g. a voided control rod follower. The method available in KAPER4 is based on a suggestion by Rowlands /19/. It was, however, necessary to extend the method for multiregion configurations. Assume a cylindrical supercell, (NR regions) where the inner NR-1 regions are a cylindrical representation of the singularity, and the outermost region consists of homogeneous core material. One calculates the axial cell diffusion coefficient from the Benoist formula

$$D_z = \frac{\sum_i v_i \phi_i \sum_j P_{ij,z}/\Sigma_j}{3 \sum_j v_j \phi_j} \qquad (6.7)$$

with volumes $V_j$, fluxes $\phi_j$, transport cross sections $\Sigma_j$, and directional collision probabilities $P_{jiz}$ /10/. Note that this buckling-independent equation is a good approximation even for voided singularities, because no planar void regions occur /19, 20/. Therefore, using eq. (6.7) for singularities is consistent with treating the leakage in the KAPER4 cell calculations.

As was shown in /9/, one can uniquely assign an axial diffusion coefficient to region j of the singularity,

$$ D_{jz} = \frac{1}{3 V_j \phi_j} \sum_i V_i \phi_i P_{ij,z} / \Sigma_j \qquad (6.8) $$

which gives the axial current when multiplied by the flux gradient. Clearly, $D_z$ in eq.(6.7) is the flux-volume average over $D_{j,z}$. The quantities (6.8) are used in the singularity option because they can be meaningfully averaged over parts of the supercell Note that the quantities used in the cell version,

$$ \tilde{D}_{jk} = \frac{1}{3} \sum_i P_{ji,k} / \Sigma_i \qquad (6.9) $$

are simpler to use, but do not have a direct physical meaning.

Following Rowlands /19/, we now set $D_N = 1/(3\Sigma_{NR})$, and attempt to determine effective $D_j^{eff}$ (j = 1,...,NR-1) such that the total leakage in the supercell is preserved; that is

$$ D_z = \left( \sum_{j=1}^{NR-1} V_j \phi_j D_{jz}^{eff} + \frac{V_{NR} \phi_{NR}}{3 \Sigma_{NR}} \right) \Big/ \sum_{j=1}^{NR} V_j \phi_j \qquad (6.10) $$

Thus, we have the requirement

$$\sum_{j=1}^{NR-1} \upsilon_j \phi_j \mathcal{D}_{jz}^{eff} = \sum_{j=1}^{NR-1} \upsilon_j \phi_j \mathcal{D}_{jz} + \upsilon_{NR} \phi_{NR} \left( \mathcal{D}_{NR,z} - \frac{1}{3 \Sigma_{NR}} \right) \qquad (6.11)$$

Note that the term in parenthesis can be written

$$\mathcal{D}_{NR,z} - \frac{1}{3 \Sigma_{NR}} = \sum_{j=1}^{NR-1} \frac{\upsilon_j \phi_j P_{jNR,z}}{3 \upsilon_{NR} \phi_{NR} \Sigma_{NR}} + \frac{P_{NR,NR,z} - 1}{3 \Sigma_{NR}}$$

and, observing that

$$P_{NR,NR,z} = 1 - \sum_{j=1}^{NR-1} \frac{\upsilon_j \Sigma_j P_{jNR,z}}{\upsilon_{NR} \Sigma_{NR}}$$

one has

$$\mathcal{D}_{NR,z} - \frac{1}{3 \Sigma_{NR}} = \frac{1}{3 \upsilon_{NR} \phi_{NR} \Sigma_{NR}} \sum_{j=1}^{NR-1} \upsilon_j \phi_j \left( 1 - \frac{\Sigma_j \phi_{NR}}{\Sigma_{NR} \phi_j} \right) P_{jNR,z} \qquad (6.12)$$

It is now obvious that the requirement (6.11) is fulfilled if we set ($j \leq NR-1$)

$$\mathcal{D}_{jz}^{eff} = \mathcal{D}_{jz} + \frac{P_{jNR,z}}{3 \Sigma_{NR}} \left( 1 - \frac{\Sigma_j \phi_{NR}}{\Sigma_{NR} \phi_j} \right) \qquad (6.13)$$

In this expression, $D_{jz}$ relates to the true axial current in region j, whereas the second term compensates for replacing $D_{NR,z}$ by $1/(3\Sigma_{NR})$. Note that (6.13) holds also if region NR extends to infinity. In the case of a two-region cell, (6.13) reads

$$D_{1z}^{eff} = \frac{1}{3\Sigma_1}\left(1 - (1 - \frac{\Sigma_1\phi_2}{\Sigma_2\phi_1})(1 - \frac{\Sigma_1}{\Sigma_2})P_{12,z}\right) \tag{6.14}$$

This expression is quoted by Rowlands for the special case when the fluxes are equal, i.e. $\phi_2 = \phi_1$.
Note that $P_{12,z}$ is calculated by the collision probability routine ACYL, which is incorporated in KAPER4. It may be useful to quote a few results for the case of a low-density channel studied by Rowlands, namely $r_1 = 5$ cm, $\Sigma_2 = 0.223$ cm$^{-1}$, $\Sigma_1$ variable. It is assumed that $\phi_2 = \phi_1$.

| $\Sigma_1$ | $D_z$ | $D_{rad}$ | $1/3\Sigma_1$ |
|---|---|---|---|
| 0.002 | 6.12 | 4.60 | 166.7 |
| 0.006 | 5.83 | 4.49 | 55.5 |
| 0.0154 | 5.28 | 4.25 | 21.6 |
| 0.05 | 3.94 | 3.50 | 6.67 |
| 0.0898 | 3.00 | 2.83 | 3.71 |
| 0.3 | 1.079 | 1.067 | 1.11 |
| 0.4 | 0.737 | 0.695 | 0.833 |

The table shows that simple diffusion theory ($D = 1/3\Sigma$) greatly overestimates the axial leakage in the channel if the density is low. Furthermore, the axial diffusion coefficient is also overestimated if $\Sigma_1 > \Sigma_2$; this is obvious from eq.(6.14). According to Rowlands /19/ there are several possibilities to define the radial diffusion coefficient. On the other hand, radial leakage in the channel is much less important than the axial leakage, especially for a channel in the core center. Therefore, no special attention was given to calculate $D_r$; rather, the above equations

were used to find it, with the axial direction z replaced by
the radial one, r.

## Comments on the Homogenization of Absorber Rods

The comments in this Section are based on work by Rowlands and
Eaton, which was presented at a meeting on homogenization at
Lugano /21/. As the proceedings of that meeting are not widely
available, the important findings of the paper will be summarized
here.
The purpose of the procedure is to produce averaged cross sections,
of the absorber rod assembly for use in whole reactor transport
(e.g. $S_N$) calculations. Note that the diffusion approximation is
less well suited for the whole reactor calculation, and involves
additional errors, because of the large absorption cross sections
of the singularity. The homogenization is necessary because usually
the absorber region is surrounded by a sodium-steel-region, and
it is not feasible to resolve the two regions in a whole-core
calculation. The fine structure of each of these regions is
neglected in this procedure.
As usual, Rowlands and Eaton treat a supercell which consists
of the absorber, the structure region, and a surrounding core
material region. They observe that the reactivity is preserved
in the homogenization procedure if the cross sections are flux-
adjoint-weighted in the following manner.

$$\overline{\Sigma} = \frac{\int d^3r \, \phi_u(r) \, \Sigma(r) \, \phi_p^+(r)}{\int d^3r \, \phi_u(r) \, \phi_p^+(r)} \tag{6.15}$$

where the flux $\phi_u$ refers to the cell with the fine structure
representation, while the adjoint flux $\phi_p^+$ must be calculated
with the cross sections of the homogenized cell. These cross
sections are not known a priori. Therefore, an iterative proce-
dure is necessary if one wants to carry out the averaging accord-
ing to eq. (6.15). Rowlands and Eaton used an $S_N$-code to perform
this iteration in one dimensional cylindrical geometry. They
assume isotropic scattering. The data are given in Table 6.1.
The important results are: If the atom densities are simply
averaged over the volume, the reactivity effect of the con-
trol rod is overestimated by 15 %, while the absorption
rate (region 1 plus 2) divided by the fission rate is overesti-
mated by 13 %.If flux-volume averaging of the cross sections is
used, the error reduces to about 5 % in the reactivity, and 4 %
in the reaction rates. This method can be considered as the first
step of the iterative procedure. It corresponds to assuming the
adjoint flux in eq. (6.15) as constant.
While there is still a systematic error, it is significantly re-
duced as compared to the simple smearing of the atom densities.
Note that the fluxes are certainly not preserved in the homogeni-
zation procedure.
In the light of these findings, the KAPER4 method can be appraised
as follows:
Clearly, a collision probability code is equally well suited for
homogenization as an $S_N$ code, with isotropic scattering. Thus,
the KAPER4 method (flux-volume weighting) is equivalent to the
first step discussed by Rowlands and Eaton. As the results of
the test example indicate, the error is expected to reduce to
about one third as compared to the simple volume averaging. Thus,
the procedure is certainly worthwhile, though there is a residual
error. The complete iteration procedure, which would reduce the
error to zero, is not possible with the present version of
KAPER4. Note that according to eq. (6.15) the radial transport
cross section should be flux-weighted in space; it is this cross
section which determines the radial diffusion into the control
rod.

Comments on the Use of the Transport Cross Sections

The singularity option of KAPER4 produces, for each region, three different types of transport cross section (or diffusion constants $D = 1/(3\Sigma_{tr})$):


- axial (parallel) transport cross section,      STR PA
- radial (perpendicular) transport cross section, STR PE
- flux-volume averaged transport cross section,   STR FV


STR PA is the effective transport cross section calculated from eq.(6.13). It is directly connected with the axial neutron leakage.

STR PE is calculated from an eq.(6.13), however, the axial collision probabilities, $P_{jNz}$, are replaced by the radial ones, $P_{jNR}$. This cross section describes the radial leakage in an infinite array of supercells.

STR FV is simply the flux-volume averaged transport cross section.

For low-density singularities (followers with/without sodium), it is obvious that the axial transport cross section, STR PA should be used. There is, however, no obvious definition for the radial transport cross section; in /19/, several possibilities are discussed, and it is observed that this quantity is not very important for a singularity at the core center. It is, therefore, recommended to use STR PE, which gives the correct leakage for singularities in a flux gradient.
For absorber rods, the situation is somewhat different. The expression for the axial leakage, eq.(6.13) in the two-region case, was derived from the condition that the axial leakage from the supercell, calculated according to Benoist, is correctly described if the singularity is assigned the diffusion coefficient $D_z^{eff}$, while the core environment has $1/(3\Sigma_{tr2})$. While this equation was derived with a low-density singularity in mind, it is still correct for an absorber singularity. However, the diffusion constant $D_z^{eff}$ can be negative in the low-energy groups, where the absorption cross section is large. This is seen immediately from eq. (6.14), if one assumes $\Sigma_1 > \Sigma_2$, and $\phi_1 < \phi_2$. The physical reason

is that the nearby absorber leads to a reduction of the axial
current in the core region. Thus, the diffusion constant
$1/3\Sigma_{tr2}$ of the core region may be too large, and must be corrected
by a negative "effective" diffusion constant of the absorber
region.

While this is physically correct, the use of negative transport
cross sections in neutronics codes is inconvenient. On the
other hand, in SNR-type cases, negative cross sections are cal-
culated only for low-energy groups, where the leakage is com-
pletely negligible. Therefore, KAPER4 does not apply this model
any more if the cross section becomes negative; rather, the
flux-volume averaged transport cross section, is then used.

The user has two options for the axial leakage:

STR PA, which is based, over most of the energy range, on Rowland's
model /19/, but the value in the low-energy groups may not be
consistent with it. Thus, if consistency is an important point
(even in energy groups where nothing happens), or the spectrum
is unusually soft the user can choose STR FV instead of STR PA.

For the radial leakage, one should use the cross section STR FV,
which describes the reactivity effect associated with the intra-
cell neutron transport correctly. The reason is that the intra-
cell leakage (from the core region into the absorber) is much
more important than the global radial leakage, in the case of
absorber rods. This point was not realized at KfK until recently.
Therefore, earlier KAPER calculations for absorber cells fre-
quently used STR PE for the radial leakage in critical assemblies
simulating an SNR-type reactor /23/. To assess the magnitude
of the error due to this point, a comparison calculation was
carried out.

For a shim-shutdown rod of the SNR-3OO (RTE, absorber part),
KAPER4 calculations were carried out, where the control rod
was surrounded by an 8 cm thick region of core material, C1.
Both a heterogeneous and a homogeneous representation of the
control rod were used.

In addition, one dimensional diffusion calculations were per-
formed in the same geometry, with cross sections prepared by

KAPER4. The resulting $k_{eff}$, using either STR FV or STR PE
are

|  | STR FV | STR PE |
|---|---|---|
| Heterogeneous RTE | 0.969204 | 0.969154 |
| Homogeneous RTE | 0.944749 | 0.944749 |
| Heterogeneity effect | 0.024455 | 0.024405 |

The calculated heterogeneity effect is nearly the same.
Therefore, the earlier calculations with STR PE are still
valid, although the theory suggests that STR FV should be used.

This section is concluded with a final remark: With the singula-
rity option, one should preferably use the KAPER4 cross sections
directly in a whole-core calculation, rather than starting out
from GRUCAL cross sections, and applying a heterogeneity correction
("KAPER heterogeneous minus KAPER homogeneous") to them.
The reason is that the case "KAPER homogeneous" is not easily
obtained for a singularity. It must be comparable to GRUCAL,
except for the different treatment of resonance self-shielding.
The best possible way to obtain self-shielded cross sections
for this case might be an arrangement where the innermost absorber
region is surrounded by several regions of the same composition.
Then, the cross sections of that innermost region are practically
only influenced by this particular composition, and may be used
as "quasi-homogeneous" data. However, as mentioned above, it is
preferable to avoid the "difference method", and to use the
KAPER cross sections directly in the SIGMN block.

## 6.3 Other Options

### 6.3.1 Reaction Rate Edits

For the comparison of experimental data with cell calculations averages of reaction rates, i.e. neutron flux multiplied by effective cross sections, over some regions of a unit cell or the whole cell volume are required. For that purpose a variety of averaging procedures is provided in KAPER4. The options available are described in 7.4.

### 6.3.2 Combination of Corrections for Heterogeneity

Repeated application of heterogeneity corrections on a given group cross section set originally created in a GRUCAL-calculation /22/ may be desirable for the approximate treatment of complicated problems of heterogeneity, e.g. the successive treatment of the heterogeneity of a pin cell and of a fuel element wrapper enclosing several of these pin cells. In such cases it may be incorrect to apply repeatedly the formula

$$\Sigma_{corr.} = \Sigma_{uncorrected} + \Sigma_{KAPER\ heterogeneous} - \Sigma_{KAPER\ homogeneous} \tag{6.16}$$

because of small differences in the number densities to be used for the calculation of the homogenized super-cell with GRUCAL and the KAPER4-calculations for the heterogeneous simple unit cell. An alternative is provided for the heterogeneity correction in such cases, which can be used instead of eq. (6.16). By choosing the input parameters MSIG,MCHI < 0 (in 7.11.5) the correction formula automatically used in the data manipulation process SIGMUT becomes

$$\Sigma_{corr.} = \Sigma_{uncorrected} \times \Sigma_{KAPER\ heterogeneous} / \Sigma_{KAPER\ homogeneous} \tag{6.17}$$

For small corrections in simple one-dimensional geometry eqs. (6.16) and (6.17) yield the same result to first order, in cases of pronounced heterogeneity the application of the cor-

rection procedure becomes questionable in any case. Eq. (6.17) can be applied if number densities used in the KAPER4-calculations are not in complete agreement with those used in the GRUCAL-calculations.

If a region of a reactor is made up of unit cells of several different types, e.g. a mixed pin cell lattice, a heterogeneity correction can be made by repeated application of eqs. (6.16) or (6.17) with fractions only of the heterogeneity correction calculated for each type of cell. Appropriate factors F for microscopic and macroscopic effective cell cross sections, for the diffusion coefficient and for the fission spectrum are input (7.11.5, K7A). The sequence of corrections to be applied to a GRUCAL group cross section set in the case of a lattice composed of cell type 1 (fraction F1) and cell type 2 (fraction F2) may be:

$$\Sigma_{corr.1} = \Sigma_{GRUCAL} + F1 \times \Sigma_{KAPER\ het.1} - F1 \times \Sigma_{KAPER\ hom.1}$$
$$\Sigma_{corr.1+2} = \Sigma_{corr.1} + F2 \times \Sigma_{KAPER\ het.2} - F2 \times \Sigma_{KAPER\ hom.2}$$
$$(6.18)$$

However, it may be necessary to account for additional restrictions prior to these corrections: The requirement of almost identical average neutron spectra in both types of unit cells of a mixed pin lattice can - as an example - be dealt with in an approximative manner by surrounding each type of unit cell by a large sea of homogenized composition already in the KAPER4-calculations. For corrections according to eq. (6.18) the averaging of cell cross sections in the KAPER4-calculations is then confined to the regions of the central unit cell with group fluxes of the super-cell taken for normalization (see 7.4.2). The validity of such approximations is not subject of this report but has to be studied by the user in each case.

## 6.3.3 Unit Cells Containing Moderator

In the latest version 1.5 of KAPER4 upward scattering in energy is permitted. It has been used for the calculation of tight

lattices of advanced pressurized water reactors currently investigated. But it should be kept in mind that some approximations inherent in KAPER4 may limit the applicability of this code:

- Scattering is assumed to be isotropic in the laboratory system. This is certainly a poor approximation for collisions of a neutron with hydrogen. A qualitative indication of the error introduced by this approximation can be obtained by calculating the collision probabilities using the transport cross section $\Sigma_{tr,g}$ (STR) instead of the total cross section $\Sigma_{t,g}$ (STOT). For reasons of consistency the within group scattering element $\Sigma_{s,g \to g}$ (SMTOT($g \to g$)) has to be modified in these cases, too:

$$\Sigma_{s,g \to g} \implies \Sigma_{s,g \to g} - \Sigma_{t,g} + \Sigma_{tr,g}.$$

This substitution may yield $\Sigma_{s,g \to g} < 0$, which is tolerated by the program. For the calculation of the diffusion coefficient and $\Sigma_{tr,g}$ anisotropic scattering is always accounted for by the usual transport approximation.

In the example given in Tab. 8.3 the influence of the substitution of $\Sigma_{t,g}$ by $\Sigma_{tr,g}$ has been calculated for the unit cell of an advanced PWR. It is negligible compared with other uncertainties of the calculation, e.g. the choice of the background cross section in the cross section preparation routine. Thus, although isotropic scattering is a poor approximation it turns out that its influence on $k_\infty$ and $k_{eff}$ is very small.

- Some approximations in the cross section preparation route are valid for narrow resonances only. These may be inadequate in cases where resonance widths are not small compared with the average energy loss in a collision or where the resonance energy is close to an energy group boundary. In such cases the validity of the approximations has to be scrutinized.

# 7. Input Description of the KAPROS module KAPER4

## 7.1 General Remarks

KAPER4, Version 1.5, is a KAPROS module /24/ written in FORTRAN 77. It replaces the KAPER program /1/ and its KAPROS-version KAPER. An input check is performed by the module PRKAP4. Compared with KAPER the new options of KAPER4 are:

- The module is a member of the KAPROS program system. Its output can be used in succeeding job steps.

- The calculation of cylindrical unit cells is possible.

- Input cross sections are read from a GRUBA file /25/, while KAPER required cross sections given in the obsolete GROU-CO-file format.

- The treatment of self-shielding, (n,2n)-reactions, elastic and inelastic scattering has been improved.

- Upward scattering and scattering beyond the energy limits of the neighbor energy group are permitted.

- Cross sections of singularities can be calculated.

- Output cell cross sections can be collapsed over several energy groups.

- Many reaction rate edits are optional.

## 7.2 Authors of the Code

The coding of the present version of KAPER4 was completed by R. Böhme and E. A. Fischer. Many subroutines are taken from

KAPER, coded by P. E. McGrath. Predecessors of some subroutines were programmed by D. Wintzer, G. Bruhn and R. Kiesel.

## 7.3 Call Parameters

The first call parameter is interpreted as the data block index IND of the input block 'KAPER_INPUT_____'. Default value is IND=1. It can be set to IND=indi by an appropriate call of the module, e.g.

*GO SM=KAPER4,MPARM=indi.

## 7.4 Task of the Module

### 7.4.1 Calculation of Eigen Value, Flux and Adjoint

The module permits the calculation of eigen value, real and adjoint flux of a fast reactor unit cell in plate geometry or cylindrical geometry. The solution of the problem can be used for the calculation of reaction rates and cell averaged cross sections. The calculation of the adjoint may follow a calculation of the real flux. It yields two sets of distributions, with the physical interpretation as importance of colliding neutrons and importance of source neutrons. The first quantity is adjoint to the flux multiplied by the total collision operator, the second one is adjoint to the flux multiplied by the production operator. In standard diffusion and transport codes the importance of source neutrons is usually calculated, while in KAPER and former versions of KAPER4 the importance of colliding neutrons was calculated.

### 7.4.2 Averaging of Cross Sections

One of the main applications of KAPER4 is the calculation of averages of group fluxes and cross sections over the cell volume or part thereof. In addition, cross sections in certain regions of the cell are required for the analysis of measure-

ments.  For that reason a variety of averaging procedures is provided in the evaluation part of the phase FLUX. Calculated quantities are:

Volume and number densities:

$$V = \Sigma_{i=j,k}(V_i)$$

$$N_\nu = \Sigma_{i=j,k}(V_i N_{i,\nu})/V$$

where i,j,k identify regions of a unit cell,

$V_i$     volume of region i;

$V$     total volume of the regions i=j,k

      (j = 1 and k = NR for the whole cell);

$N_{i,\nu}$     number density of an isotope $\nu$ in region i;

$N_\nu$     average number density of an isotope $\nu$ in V.

Volume averages of the group fluxes over the whole cell or parts of the cell:

$$PHI_g = \Sigma_{i=j,k} (V_i\ PHI_{g,i}) / V$$

where g is an energy group number,

$PHI_{g,i}$ neutron flux density in group g and region i;

$PHI_g$    average neutron flux density in group g,

      regions i=j,k.

Flux×volume averages of macroscopic and microscopic cross sections over the whole cell or parts of the cell:

$$SIGMA_{g,\nu} = \Sigma_{i=j,k} (V_i\ PHI_{g,i}\ SIGMA_{g,i,\nu}) / (V\ PHI_g)$$

$$sigma_{g,\nu} = SIGMA_{g,\nu} / N_\nu$$

where

  $SIGMA_{g,i,\nu}$ macroscopic cross section in group g, region i, isotope $\nu$;

  $SIGMA_{g,\nu}$ averaged macroscopic cross section in group g, isotope $\nu$;

  $sigma_{g,\nu}$ averaged microscopic cross section in group g, isotope $\nu$.

Special flux×volume averages of cross sections over parts of the cell (l=m,n), but normalization made with the volume averaged flux ($PHI_g$) of the whole cell:

$$SIGMA'_{g,\nu} = \Sigma_{l=m,n} (V_l \ PHI_{g,l} \ SIGMA_{g,l,\nu}) / (PHI_g \ \Sigma_{l=m,n}(V_l))$$

This option can be used for the simulation of multi-cell problems.

Special flux weighted microscopic cross sections for the analysis of reaction rate measurements:

$$srate_{g,i,\nu} = (sigma_{g,i,\nu} \ PHI_{g,i}) / PHI_g$$

where $sigma_{g,i,\nu}$ are microscopic cross sections in group g, region i, isotope $\nu$; and $srate_{g,i,\nu}$ are microscopic cross sections containing the information about flux fine structure. srate multiplied by fluxes of global rector calculations yields a fine structure corrected reaction rate distribution.

Adjoint or bilinear weighted quantities are not provided by the program.

7.4.3 Cross Sections of Singularities

KAPER4 can be used for the calculation of effective cross sections of singularities, i.e. control rods, followers, etc. The method is described in 6.2.

### 7.4.4 Collapsing of Cross Sections

Provision is made to collapse effective group cross sections of the cell and capture and fission cross sections in selected regions from the group structure used in the KAPER4 calculation into a new group structure with less groups prior to output. The real fluxes calculated for each region of the unit cell are used as the weighting function for this procedure. Collapsing with other weighting functions is not programmed. For all cross sections weighting with the product of flux and volume is carried out.

### 7.4.5 Inhomogeneous Problems and Perturbation Calculations

In plate geometry inhomogeneous problems can be solved and perturbation calculations can be carried out, see 6.1.

### 7.5 Method of Solution

Self-shielded region-wise cross sections are calculated by the method of Wintzer /2/. Using these cross sections, an eigen value problem in plate or cylindrical geometry is solved by the collision probability method. In plate geometry this method is also applied for the solution of boundary source problems and perturbation calculations using exact perturbation theory.

The test module PRKAP4 is only used for the examination of input data and the calculation of storage space required.

### 7.6 Restrictions

### 7.6.1 Limits of Application

The test module PRKAP4 confines input testing to a maximum number of 150 different isotopes. If more isotopes are used in

a unit cell, a dummy test module (e.g. PRDUM) has to be called. This has no effect on calculated results.

There are inherent limitations in the theoretical formulations which may restrict the applicability of the code. These are:

- Scattering is assumed to be isotropic in the laboratory system. A transport-correction is always applied for the calculation of the diffusion coefficient. The use of transport cross sections instead of total cross sections for the calculation of collision probabilities is optional.

- Cross sections have to be provided as unshielded infinite dilution cross sections plus shielding factors (frequently called f-factors) at fixed temperatures for all materials constituting the cell. Temperature interpolation of cross sections is not possible (see 7.11.4, K5). f-factors > 1. are not permitted by the interpolation routine. Therefore, a warning is printed in these cases and the factors are set =1. The user has to decide about the adequacy of this approximation.

- Solutions of inhomogeneous problems and perturbation calculations in cylindrical geometry are not possible.

### 7.6.2 Boundary Conditions (see Fig. 7.1):

7.6.2.1  Plate geometry (Input parameter KGEO = 1)

The program assumes periodic boundary conditions in the direction perpendicular to the plates. Reflective boundary conditions have to be simulated by adding a mirror image of the cell, thus doubling the number of regions. Infinite extension of the plates is assumed in two orthogonal directions (see Fig. 7.2).

7.6.2.2 Cylindrical geometry (Input parameter KGEO ≥ 2)

An infinite hexagonal or square lattice of cells is assumed.
The cell extends to infinity in the direction of the main axis.
The cell may be approximated by an equivalent circular cylinder
(KGEO = 2, Wigner-Seitz-Cell) with white boundary conditions
(see 5.2) at the outer surface. Alternatively a square (KGEO =
3) or hexagonal (KGEO = 4) outer cell boundary is assumed. The
collision probabilities for neutrons entering (or produced in)
the outer region are then calculated using an approximation of
Sauer /16/.

7.6.3 Numerical Uncertainties

The neutron optical thickness of any region (i.e. total macro-
scopic cross section multiplied by the thickness) should not
be smaller than $10^{-4}$. This restriction implies that a region
may not be truly voided. Simulated void-regions should contain
typically approximately $10^{20}$ atoms/cm$^3$ of some inert material
(e.g. Fe, O, etc). A general rule for these cases cannot be
given. A violation of limits can be easily detected by vari-
ation of the void-simulation and observation of calculated
parameters. The uncertainty of the final eigenvalue will be
about 10 times the uncertainty EPSPHI requested in the input,
K3 of phase FLUX. The k-value calculated from a reaction rate
balance after the final iteration may also differ from the
eigenvalue by 10×EPSPHI. The lower limit is always $\geq 10^{-5}$.

The accuracy decreases with increasing number of regions and
energy groups due to the cumulation of numerical uncertainties.

7.6.4 Correction for Leakage

A correction for leakage can be achieved by scaling collision
probabilities in each energy group by $(1 + (D \times B^2)/SIGT)^{-1}$,
where SIGT is the total group cross section in the unit cell,

D is the diffusion coefficient calculated for the lattice and $B^2$ are input bucklings. If the corrections $|D \times B^2/SIGT|$ exceed 0.2 in any energy group a warning is printed in the output, but the problem is solved in the usual manner. Negative bucklings for leakage correction are permitted. However, if convergence to an eigen value is not achieved by the usual reduction of collision probabilities a warning is issued and an attempt is made to solve the problem with a leakage correction (1 - $(D \times B^2)/SIGT$) of the collision probabilities. In such cases and in cases where elementary diffusion theory is inapplicable because of high absorption the method of correction for leakage may be inappropriate.

The eigen value $k_{eff}$ is a function of the input bucklings via the leakage correction. The code contains an option to modify the bucklings, in an iterative procedure, such that a desired value of $k_{eff}$ is obtained.

## 7.7 Typical Running Times on a Siemens M7890

For problem examination and termination because of input errors CPU-time is < 1 sec. Solution of a typical 3 region cell problem for 26 or 69 energy groups requires a total CPU-time of < 10 sec. For the solution of a 16 region cylindrical cell problem for 69 energy groups the CPU time increases to ≈300 seconds.

## 7.8 Special Applications

### 7.8.1 Cross Sections of a Singularity

It is possible to calculate effective cross sections of a singularity simulated by a cylindrical axial channel surrounded by a large sea of core material (see 6.2).

## 7.8.2 Low Density Regions

The neutron streaming effect in a low-density region (appr. $10^{20}$ atoms/cm$^3$) can be calculated with the following precautions:

- The parallel diffusion coefficient in a plate cell is overestimated if the density is too low. More accurate diffusion coefficients can be obtained by use of the program PARDON /9/.

- If the low-density region is the outermost region in a pin cell, KGEO = 3 or 4 (square or hexagonal boundaries) produces better results than KGEO = 2 (Wigner-Seitz-cell). It is recommended to use the program ARIADNE /5/ in cases of true void regions.

## 7.8.3 Homogenized Cells

To run easily a case for a homogenized cell with KAPER4, the input parameter KGEO may be given as a negative number: KGEO = -|KGEO|. In this case the geometry of the cell is maintained, but the composition of each region is replaced by that of the homogenized cell. For a cell containing a large number of regions it is recommended for the sake of shorter running time to use the number densities of the homogenized cell (output of the heterogeneous calculation) and run a case for a simplified few region cell.

The alternative method characterized by the reduction of all cell volumina to small values leads in the limit to the homogenized cell, too. Its limitations due to numerical errors are discussed in 5.1 and demonstrated in Table 8.1.

## 7.9 Support Programs Used

The KAPROS system /24/ routines needed are:
KSINIT KSDLT KSPUT KSPUTP KSGET KSGETP KSCC KSDD.

The library function MMDEI of IMSL and system functions for log, cos, exp, sqrt are used. Microscopic cross sections are read from a GRUBA-file /25/ by support of the subroutines GRU-SEEK /25/.

## 7.10 Hardware Requirements

The module length is 405 k bytes. The cross section preparation phase requires maximum storage (in bytes):

IS = 4×(106 + 8×NIS + 38×NR + 10×NR×NR + 32×NIS×NOG
        + 2×NIS×NOG×NOG + NIS×NR + NOG×NR)

where
 NIS number of isotopes in the unit cell,
 NOG number of energy groups in the microscopic cross section
        tables,
 NR  number of regions in the unit cell.

For the transition from the cross section preparation phase to the cell calculation phase and the perturbation worth phase one data set with RECFM = VBS of the length LU = 4×((5 + NR)×NOG×NOR + (2 + NOG)×NFI + 5×NR + 4) bytes is required.
 NOR = number of isotopes for reaction rate calculations
 NFI = number of fissionable isotopes in the cell

For each perturbation sample to be inserted in the unit cell a data set of similar length is required. If optional output is requested (cell averaged number densities, bucklings after criticality search), formatted output is written with LRECL = 80 on a unit selected by the user.

## 7.11 Coding of the Input Data

### 7.11.1 Dimensions and Normalization

All dimensions are omitted in the output of KAPER4. The user has to take care of the proper selection of dimensions via input. The relations between the dimensions of the KAPER4 input quantities microscopic cross section /sigma/, number density /N/, length /L/ and bucklings /B²/ must be

$$/L/ = /\text{sigma}/^{-1} \times /N/^{-1}$$
$$\text{and} \quad /B^2/ = /\text{sigma}/^2 \times /N/^2$$

Two examples of widely used systems are given in Tab. 7.1. The classical version is standard with GRUBA-files. Time dependence is not considered. Energy dependence is treated by the multi-group method. Temperatures have to be given in units requested in the input description (Kelvin for the cell temperature, MeV for the calculation of fission spectra).

Region volumes $V_i$ (i = 1,NR) are calculated according to the geometry option chosen. Input quantities are the thicknesses $T_i$ shown in fig. 7.1. With $R_i = \Sigma_{j=1,i} T_j$, $R_0 = 0$ the volumes are:

- plate geometry:
  KGEO = 1 $\qquad V_i = T_i \times /L/^2$ $\qquad\qquad$ i = 1,NR

- cylindrical geometry, circular outer boundary:
  KGEO = 2 $\qquad V_i = \pi \times (R_i^2 - R_{i-1}^2) \times /L/$ $\qquad$ i = 1,NR

- cylindrical geometry, square outer boundary:
  KGEO = 3 $\qquad V_i = \pi \times (R_i^2 - R_{i-1}^2) \times /L/$ $\qquad$ i = 1,(NR - 1)

  $$V_{NR} = (4 \times R_{NR}^2 - \pi \times R_{NR-1}^2) \times /L/$$

- cylindrical geometry, hexagonal outer boundary:

KGEO = 4 $\qquad V_i = \pi \times (R_i^2 - R_{i-1}^2) \times /L/ \qquad i = 1,(NR - 1)$

$$V_{NR} = (3.4642 \times R_{NR}^2 - \pi \times R_{NR-1}^2) \times /L/$$

The calculated flux densities are normalized to produce 1 neutron (per time unit) in the unit cell:

$1 = \Sigma_i \ V_i \ \Sigma_g \ PHI_{g,i} \times (NU \times SFISS)_{g,i}.$

The calculated adjoint (importance of colliding neutrons, ADPHI) is normalized to yield a produced worth equal to $k_{eff}$:

$k_{eff} = \Sigma_g \Sigma_i \ CHI_{g,i} \times ADPHI_{g,i} (\Sigma_{g'} \ (NU \times SFISS)_{g',i} \times PHI_{g',i} \times V_i)$

where $\Sigma_i$ = summation over all regions i = 1,NR

$\qquad \Sigma_g$ = summation over all energy groups g = 1,NOG

$\qquad$ CHI $\quad$ = fission neutron spectrum

$\qquad$ NU $\qquad$ = number of neutrons produced per fission

$\qquad$ SFISS = fission cross section

## 7.11.2 External Units

It is possible to store the region cross sections calculated in phase SSXS as a permanent data set for repeated later use in the cell calculation phase FLUX.

Note: After a calculation of the adjoint the cross sections stored in a data set in phase SSXS are altered in order to permit a perturbation calculation. They cannot be used for a second phase FLUX calculation.

The formatted output - in the example collected on unit no. 10 - can conveniently be stored as a data set for later manipulations. For most applications within the KAPROS-system data transfer can be made via KAPROS data blocks.

7.11.3 Input Sequence of the KAPROS Block 'KAPER INPUT     '

The block may be given as a KAPROS external block.

Remark: Character expressions are identified by the number of characters in each string (4 or 8). If an expression is a constant, it is given between a leading and a trailing apostrophe ('), as required in a KAPROS external block. Further, _ stands for blank, | | for the absolute value and / / for the dimension of a quantity.

The program is subdivided in 3 subtasks (i.e. phases). The phases can be called by their identifying key word. A logical order should be obeyed, i.e. data requested by a certain phase have to be calculated prior to its execution or given as input data via an external data set.

For historical reasons the grouping of input parameters on cards K is maintained in the present description. Only in a few cases is the sequence of data different from former versions of KAPER. Old input card decks can be used with little or no changes.

7.11.4 Phase SSXS, Cross Section Phase

In this phase the resonance self-shielded cross sections for each region of the heterogeneous cell are calculated and stored in external data sets for use in subsequent phases.

| K1 | 'SSXS' | CHARACTER*4, key word |
|----|--------|----------------------|
| K2 | GRSN | CHARACTER*8 |
|    |        | Group cross section set name, e.g. 'KFKINR__' |
| K3 | NOG | Number of energy groups |
|    |        | Note: Numbering of groups should be ascending with decreasing energy. |
|    | NB | Number of terms (recommended NB = 6) in the |

approximation of the reaction coefficients
by a series of rational functions.

KGEO       < 0     The problem will be solved with region
number densities replaced by those of the
homogenized cell.

|KGEO| = 1 Plate geometry

          = 2 Cylindrical geometry with outermost
               cylindrical boundary and white
               boundary conditions

          = 3 Cylindrical geometry with outermost
               square boundary

          = 4 Cylindrical geometry with outermost
               hexagonal boundary

IHI        IF IHI > 0, number densities of the homogenized
unit cell will be written on unit IHI in the
format suitable for GRUCAL /22/ input.
(LRECL ≥ 80, RECFM = FB, DD-card required)

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 for
the isotopes specified by IS(i) (see K9).

NCHI      |NCHI| ≤ 10
If NCHI = 0, the internal fission neutron
spectra (see K10) are used in all calculations.
If NCHI > 0, it specifies the number of
fissionable isotopes for which a fission
spectrum is read in as input (cards K10 and
K11).
If 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 from that of
               the Karlsruhe sets,

           2 - the temperature of the Maxwellian
               distribution is to be changed from that
               given internally in the program (see K10).


ITRANS     ITRANS = 0 normally;

              if ITRANS < 0, total cross sections will be
              replaced by transport cross sections and the
              diagonal term of the scattering matrix will be
              corrected accordingly prior to writing cross
              sections on unit NAP.


K4    GAM      Parameter for the approximation of cross
              sections.  Recommended is GAM = 1000. (see
              4.1).


    EPS      Parameter as above, recommended  is EPS = 0.


K5    NIS      Total number of isotopes
    (ISOT(i), TEMPT (i), i=1,NIS)
              Isotope names (CHARACTER*8) as specified by
              the convention of the cross section set, and
              temperatures of the isotopes in Kelvin. The
              temperatures must be identical to one of the
              standard temperatures at which self-shielding
              factors are stored in the cross section file.
              Temperature interpolation is presently not
              possible.


K6    NISS     Number of isotopes, for which self-shielding
              should be neglected.
    If NISS > 0:
    (ISON(i),i=1,NISS) Isotope names (CHARACTER*8)

K7    NR           Number of regions into which the cell is divided (NR ≥ 2).

(T(i),i=1,NR)    Thickness of the $i^{th}$ region.

(MIX(i),i=1,NR)  Mixture number of the $i^{th}$ region as determined by the order j in card K8.

K8    NMIX        Number of different mixtures

((CON(j,i),i=1,NIS),j=1,NMIX)    Isotope concentration

K9    MPERT       = 0, if the cross sections are being prepared for the calculation of fluxes of the normal core cell in phase FLUX.
                     = 1, if the cross sections are being prepared for reactivity worth calculations in phase PERT or for the perturbed cell option in phase FLUX.

       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 SSXS calculation. In this manner the cross sections for reactivity worth samples can be stacked one after the other on the same unit.
                     - Include DD-card for unit NAP (RECFM=VBS) -

If (NOR = 0), go to S1

     (IS(i),i=1,NOR)  Number of the isotope in the ISOT(i) array for which reaction rate cross sections are desired.

S1    If NCHI = 0, end of card input for phase SSXS.
       If NCHI > 0, go to K10
       If NCHI < 0, go to K12

(Cards K10 and K11 are repeated NCHI times)

K10  NAME          CHARACTER*8,  Name of fissionable isotope for
                   which a fission neutron spectrum is to be read
                   as input. The characteristic temperatures of
                   the 10 standard fission spectra in KAPER4 are
                   given in Tab. 7.2.  The program also
                   associates isotope names given in the last
                   column of Tab.  7.2 with standard fission
                   spectra. However, these names cannot be used
                   for the identification of a spectrum to be
                   altered or replaced.

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

S2   End of card input for phase SSXS.

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

     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 S4

K13  N             Number of new energy limit values to be
                   read in (N ≤ NOG of K3).
     (E(k),k = 1,N)  Upper energy limit of the k$^{th}$
                   energy group in MeV.
                   Note: Contributions to CHI in the range < 1 keV
                   are collected in the last energy group with
                   E(k) > 1 keV.  Contributions to CHI from the

range 20 MeV to E(1) are collected in group 1.

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

(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 SSXS.

## 7.11.5 Phase FLUX, Flux, Adjoint and Reaction Rate Phase

In this part 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 SSXS.

K1  'FLUX'      CHARACTER*4, key word

K2  NHOM        = 0 Recommended.
                > 0, if the user wishes to use the collision probabilities from phase SSXS (transfered on unit NAP, NXST, resp.). If the thickness of the plate cell is near the lower limit of the validity of the method, this option may improve slightly the accuracy of the results.

NXST        Number of an external unit which contains cross sections for the normal cell (a unit NAP of phase SSXS). 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 PERT. If
NXST is negative, the adjoint distribution in
the cell is not calculated.

Note: After a calculation of the adjoint the cross sections
stored on unit NXST in phase SSXS are altered in order to permit
a perturbation calculation. They cannot be used for a second
phase FLUX calculation.

NPERT      Valid for slab geometry only.
                 Number of an external unit which contains cross
                 sections for the perturbed cell (a unit NAP of
                 phase SSXS). 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, from the
                 normal cell.
                 If 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
                           (input K4A or K4B)
            > 1      Group dependent bucklings to be used
                           (input K5A or K5B)

KBSQ        > 0: Iteration on bucklings to a desired
                 $k_{eff}$ as specified on card K6. After the
                 iteration new bucklings are stored in the
                 KAPROS block 'KAPER_BUCKLINGS_'.
                 = 0 Otherwise.

NGC    =1    Valid for plate geometry only!
If the perturbed cell, as defined on unit
NPERT, is to be extended by a normal cell from
unit NXST on each side before calculation of
the flux distribution in the perturbed cell.
This option can be used to investigate the in-
fluence of the perturbed cell boundary selec-
tion without redefining the cell in phase SSXS.
= 0   For all other cases.


IAN    = 2   Anisotropic leakage is considered and
directional diffusion coefficients will be
calculated. If this option is selected,
bucklings should be input (K4B or K5B). The
diffusion coefficient is calculated parallel
and perpendicular to the main axis as indicated
in Fig. 7.2.
= 1   As above, but STR_PE is calculated from
the quantities STR and STR_PA. This option
should not be used in the case of cylindrical
cells.
= 0   Otherwise


IHCS   ≠ 0   Option to homogenize cross sections
over part or all of the regions in the basic
unit cell for use in a succeeding calculation.
To produce average cross sections for a (cylin-
drical) singularity, it is required to put
|IHCS|=NR-1 and KGEO ≥ 2, and to fill region NR
with core material (thickness of the order of
two mean free paths). |IHCS| ≠ NR-1 otherwise.
IHCS < 0   permits the output of fractions of
KAPER4- cross sections into the blocks
'INPUT SIGMUT$$$' for the approximate solution
of multi-cell problems.
= 0 Otherwise

K3   IMIN        Minimum number of outer iterations for convergence on the eigenvalue (IMIN ≥ 3).

     IMAX        Maximum number of outer iterations, e.g. 20.

     EPSPHI     Convergence criterion for the fluxes, EPSPHI ≥ $1 \times 10^{-6}$.

     EPSKEFF    Convergence criterion for the eigenvalue $k_{eff}$, EPSKEFF ≥ $1 \times 10^{-6}$.

Note: Due to numerical errors the uncertainty of the eigenvalue is about 10×EPSPHI.

S1    If  IB = 0, go to S3
     If  IB > 1, go to S22

S21   IF  IAN > 0, go to K4B

K4A   BSQ        Universal buckling, isotropic and independent of group number.
     Go to S3

K4B   BSQPARA, BSQPERP   Universal bucklings in two directions, independent of group number, see Fig. 7.2.
     Go to S3

S22   If IAN > 0, go to K5B

K5A   (BSQ(k),k=1,NOG)  Isotropic and group dependent bucklings, NOG = number of energy groups.
     Go to S3

K5B   (BSQPARA(k),k=1,NOG),(BSQPERP(k),k=1,NOG)  Group dependent bucklings in two spatial directions, see Fig. 7.2.

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

K6    MAXB        Maximum number of iterations on the bucklings to obtain the specified $k_{eff}$.

       AKE        Desired $k_{eff}$

       EBK        Maximum deviation of $k_{eff}$ from the desired value AKE.

       FAK        > 0.    Factor used to multiply the initial bucklings for a second guess (recommended 1.2)
= 0.    For a second guess all bucklings are reduced by $1 \times 10^{-3}$
< 0.    For a second guess all bucklings are reduced by |FAK|. If IAN = 1, the reduction is |FAK| multiplied by (|BSQPERP|)/(|BSQPERP| + |BSQPARA|) and (|BSQPARA|)/(|BSQPERP| + |BSQPARA|) for the appropriate direction dependent bucklings. These splitting factors are set to 1/3 resp. 2/3, if |BSQPARA| + |BSQPERP| = 0.

       NBQ        > 0    Number of a unit onto which new bucklings are written after the last iteration (LRECL ≥ 80, RECFM = F, DD-card required, if NBQ ≠ 6)
≤ 0    Otherwise

S4    If IHCS = 0  (on K2) End of card input for phase FLUX, otherwise follow input data for the output of homogenized cell cross sections.
If IHCS > 0       go to K7B
If IHCS < 0       go to K7A

K7A     Factors for the multiplication of cross
        sections prior to output into the KAPROS-block
        'INPUT_SIGMUT$$$$' *), used for the simulation
        of multi-cell problems:

| | |
|---|---|
| FAKMAC | multiplicand of macroscopic cross sections, |
| FAKMIC | multiplicand of microscopic cross sections, |
| FAKCHI | multiplicand of CHI, |
| FAKD | multiplicand of all diffusion coefficients, |
| IPRINT | no print-out of cross sections, if IPRINT = 0. |

K7B IM    |IM| number of a mixture in a SIGMN-block
        named 'SIGMN_KAPER_____' created by the module
        GRUCAL /22/.  It can be modified by means of
        the KAPROS-block 'INPUT_SIGMUT$$$$' *), which
        will be created in this phase.

        If IM < 0, group collapsing will be carried out
        (input card K9).

   IRR    If IRR ≠ 0, microscopic reaction rate cross
        sections 'SFISS___' and 'SCAPT___' for the
        isotopes (IS(i),i = 1,|IRR|) are included in
        the KAPROS-block 'INPUT_SIGMUT$$$$'. IS(i) is
        input in phase SSXS, K9. Note that for a
        modification procedure identical types
        (isotope names ending ..MIC) have to be
        included in the block 'SIGMN_KAPER_____'.

        If IRR < 0, regionwise constant reaction rate
        cross sections will be calculated in addition
        and stored in the data block
        'XS_RATES_____' (include K10). These cross

---

*) $$$$ stands for ____, HET_, or HOM_, according to MSIG

sections provide heterogeneity corrected
reaction rates in each cell region if
multiplied by cell averaged fluxes.

IRR = 0 otherwise.

IZ          Number of additional transport cross section
            types to be included in 'INPUT_SIGMUT$$$'. For
            permitted choices see TYPE of K8.

MSIG        Indicator for the intended application of the
            block 'INPUT_SIGMUT$$$$' and selection of
            $$$$:
            = 0 ($$$$ = ____) KAPER4 cross sections
            replace the cross sections of mixture |IM| in
            the SIGMN-block 'SIGMN_KAPER____'.
            = 1 ($$$$ = HET_) KAPER4 cross sections will
            be added to the cross sections of mixture
            |IM|.
            =-1 ($$$$ = HET_) KAPER4 cross sections will
            be multiplied with the cross sections of
            mixture |IM|.
            = 2 ($$$$ = HOM_) KAPER4 cross sections will
            be subtracted from the cross sections of
            mixture |IM|.
            =-2 ($$$$ = HOM_) the cross sections of
            mixture |IM| will be divided by KAPER4 cross
            sections.

Note: See 6.3.2 for hints on the proper choice of MSIG.

MCHI        = 0  KAPER4-CHI replace the CHI-data of mixture
                 |IM|.
            = 1  KAPER4-CHI will be added to CHI of mixture
                 |IM|.
            =-1  KAPER4-CHI will be multiplied by CHI of

mixture |IM|.

= 2    KAPER4-CHI will be subtracted from CHI of
mixture |IM|.

=-2    CHI of mixture |IM| will be divided by
KAPER4-CHI.

= 3    CHI will not be included in
'INPUT_SIGMUT$$$$'.

IS          |IS| Number of the first region to be included
in the homogenization procedure of cross
sections, usually |IS| = 1.

If IS < 0, K7A to K10 will be repeated after
K10. The data of this second averaging process
will be included in a further block
'INPUT_SIGMUT$$$$', IND = OLDIND + 1, with
$$$$ set according to the next choice of MSIG.
By this option several cross section
modifications can be obtained from a single
KAPER4 calculation.

IE          |IE| Number of the last region to be included
in the homogenization procedure, usually IE =
NR of SSXS(K7). If IE < 0, the averaging
procedure will be carried out for cross
sections in regions |IS| to |IE|, but
normalization will be made to the average cell
flux in regions 1 to NR. By choice of this
option the flux fine structure of the cell will
be represented in the output cross sections.

S5    If IZ = 0, go to S6
(no additional transport cross section types)

K8    (TYPE(i),i = 1, IZ)  CHARACTER*4
Permitted 'TYPE's are:

'PE$$' for perpendicular diffusion

'PA$$' for parallel diffusion (see Fig. 7.2)

'FV$$' flux and volume weighting of regionwise transport cross sections (beware of possible condensation errors, if IM<0)

'BS$$' usual STR-type of KAPER4 obtained by buckling weighting perpendicular and parallel diffusion coefficients.

'__$$' as above

'VO$$' special option for the creation of a data block 'KAPER STR VOID'. This block contains all data needed for the calculation of directional diffusion coefficients of a true two-dimensional void in a two region cell by the programs ARIADNE /5/ or PARDON /9/. Beware of the meaning of IE on K7B in this case: the cell will be divided in two parts, region 1 extending from 1 to IE, region 2 extending from IE+1 to NR.

The different types of transport cross sections will be labelled 'STR_TYPE', with $$ in the word TYPE arbitrarily chosen by the user. See 3.3 on the choice of TYPEs for diffusion or transport calculations.

Remark: A 1/3 - 2/3 weighting of directional diffusion coefficients is equivalent to 1/(3×STR) of the isotropic calculation (IAN = 0).

S6   If IM > 0, go to S7 (no collapsing of group cross sections)

K9   NG           Number of new groups (≤ number of old groups)

(NEWG(i),i=1,NG) <u>Uppermost</u> in energy - old group which

falls into new group i; NEWG(1) = 1 in general.

S7    If IRR ≥ 0, go to S8 (no microscopic cross sections in
           selected cell regions)

K10  NUT      Number of a unit onto which cross sections are
              to be written (formatted, LRECL ≥ 80,
              include DD-card, if NUT ≠ 0 or 6).

     NUK      Number of regions, for which regionwise
              microscopic reaction cross sections shall be
              calculated.

     (NRR(i),i=1,NUK)     Region numbers selected
              (1 ≤ NRR ≤ NR from K7 of phase SSXS)

S8    If IS < 0 return to S4, otherwise end of input of phase
           FLUX.

7.11.6 Phase PERT, Reactivity Worth Phase

Attention: This phase is at present only applicable to plate
           geometry, |KGEO| = 1 on card K3 of SSXS.

K1    'PERT'   CHARACTER*4, key word

K2    NFLUX    Number of an external unit containing cross
               sections and fluxes for the normal cell.
               Normally NFLUX=NXST on card K2 of phase FLUX
               after a calculation of the adjoint.

      NPERT    Number of an external unit containing cross
               sections and fluxes for the perturbed cell.
               Normally NPERT=NPERT on card K2 of phase FLUX.
               When the perturbed cell 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.

NXECT     Number of an external unit containing cross
sections for the various samples to be
calculated (a unit NAP of one of the phase
SSXS calculations).

NTAPE     Additional external unit (RECFM=VBS) for
storing collision probabilities. The space
needed on this unit is

SPACE   = $4 \times NOG \times IX \times IX$ bytes, where

  NOG    = number of energy groups

  IX      = $2 \times NCELL \times (NY + NW)$

  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    Additional external unit for storing collision
probabilities. The space needed on this unit
is the same as calculated for NTAPE, RECFM=VBS.

NSAM      Number of samples to be calculated. This is
the number of sets of group constants on unit
NXECT.

NFP       Maximum number of fissionable isotopes in any
one set of group constants on unit NXECT.

NCELL     Number of normal cells ( $\geq 1$) to be placed
on either side of the perturbed cell for the

calculation of the reactivity effects. For
this range changes in collision probabilities
will be calculated. NCELL should be large
enough so that the probability of a neutron
from the perturbed cell to suffer 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. This value is chosen to yield a neutron
optical thickness of about 6.5 of the normal
cells on either side. It depends, of course,
on the energy group.

| | | |
|---|---|---|
| K3 | IH | = 1, Flux and adjoint distributions are to be superimposed on a group-dependent cosine curve, normal to the plate cell. This curve is defined by the bucklings BSQPERP given on card K4B or K5B of phase FLUX if IAN > 0 as $f(x) = \cos(\sqrt{BSQPERP} \times x)$, if $BSQPERP \geq 0$; $f(x) = 1$, if $BSQBERP < 0$. The centre point, $x = 0$, is located at the centre 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 FLUX) 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 FLUX. = 0, Option not used =-1, A modified density can be specified in one |

or more regions of the perturbed cell with card K5.

NUNPER
If MORE = 1, number of an external unit with new cross sections and/or region dimensions for the perturbed cell as prepared from phase SSXS. 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

$$S_f(0) \times S^+(0) / \int (S_f(r) \times S^+(r)) dr,$$

where $S_f(r)$ and $S^+(r)$ are the fission and adjoint sources, respectively, and the integration is over the reactor core and reflector. The sample is assumed to be located at r = 0.

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

K5
(VOID(i),i=1,NW)  VOID(i) < 1.0 for the $i^{th}$ region in which a reduced density is simulated in the unperturbed state, otherwise set VOID(i) = 1., 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 $i^{th}$ region by simply putting VOID(i) equal to an appropriate value, e.g., to reduce the density in the $i^{th}$ 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 CHARACTER*4 words in the
                        description title (NT ≤ 15)

    (TITLE(i),i=1,NT) CHARACTER*4    Description title

End of card input for phase PERT.

## 7.12 Data Blocks Created by the Module:

### 7.12.1. Data block 'KAPER_MIX_____' :

The data block contains number densities of the homogenized unit cell. It can be included in the block MISCH of the module GRUCAL /22/.

NIS        Number of isotopes in the homogeneous mixture
6*'____'  6 words CHARACTER*4, 4 blanks each
(NAME(i),TEMP(i),CON(i),i=1,NIS)
             Name of the isotope in KAPER4-input (CHARACTER*8),
             temperature in Kelvin and number density of each
             isotope.

### 7.12.2. Data block 'KAPER_GEO_____' :

The data block contains information about the cell geometry. It must be present for a succeeding calculation of anisotropic diffusion coefficients using the module ARIADNE. It contains:

KGEO            Geometry index of KAPER4
NR              Number of regions of the unit cell
(R(I),I=1,NR)     Thicknesses of regions
(V(I),I=1,NR)     Volumes of regions

7.12.3. Data block 'KAPER_BUCKLINGS_' :

This block will only be created after an iteration on bucklings to a specified $k_{eff}$. It contains the bucklings used for the last step of the iteration.

(BSQPARA(g),BSQPERP(g),g=1,NOG)

       Two direction dependent bucklings per energy group g=1,NOG; see Fig. 7.2 for the definition of directions.

7.12.4. Data block 'XS_RATES_____' :

The datablock contains microscopic cross sections for the calculation of fine structure corrected reaction rates using the module RATES.

| | |
|---|---|
| NUK | Number of regions of a unit cell for which cross sections are provided |
| IRR | Number of materials for which cross sections are provided |
| NG | Number of energy groups in the output (NG ≤ NOG) |
| TYPE(1) | Word 'SCAPT___', CHARACTER*8 |
| TYPE(2) | Word 'SFISS___', CHARACTER*8 |
| (ISOTOP(i),i=1,IRR) | Names of the IRR isotopes i, CHARACTER*8 |
| (NRR(r),r=1,NUK) | Numbers of the NUK regions r in the unit cell |

(((scapt(g,i,r),g=1,NG),(sfiss(g,i,r),g=1,NG),i=1,IRR),r=1,NUK)

       Microscopic capture cross section scapt in each energy group g, microscopic fission cross section sfiss in each group g, for each isotope i and each region r.

7.12.5. Data block 'INPUT_SIGMUT$$$$' :

On request, data blocks 'INPUT_SIGMUT$$$$', IND ≥ 1, with $$$$ set according to 7.11.5, K7B of the phase FLUX, will be creat- ed. Each call for an averaging procedure increases the block index by the increment 1, if block names are identical. The blocks contain all input required and the cross sections to be used for the modification of a SIGMN block /22/ 'SIGMN_KAPER_____' by the module SIGMUT. The length of a block is 4×(7+(2×NG+8)×(6+NG+2×IRR+IZ)) bytes.

    NG  = number of energy groups in the output cross section file
    IRR = number of materials, for which microscopic cross
            sections for reaction rate calculations are requested
    IZ  = number of additional cross section types requested, e.g.
            direction-dependent transport cross sections.

7.12.6. Datablock 'KAPER_STR_VOID__' :

This block provides data required for an execution of the mod- ule ARIADNE /5/. It includes addresses of data to be found in 'INPUT_SIGMUT____' (MSIG=0, TYPE='VO') and transport cross sections required for the calculation of the diffusion coeffi- cients of a cylindrical cell having a true void region.

7.13 Data Blocks Read by the Module

The data block containing all input data is named 'KAPER_INPUT_____'. It can be provided as an external block with the leading information
*KSIOX DBN=KAPER_INPUT_____,IND=indi,PMN=PRKAP4,TYP=CARD
and the terminating information
*$*$
Its content is given in chapter 7.11.

The test module PRKAP4 confines input testing to a maximum number of 150 different isotopes. If more isotopes are used in a unit cell, a dummy test module (e.g. PRDUM) has to be called.

## 8. Sample Problems

The input data for three examples are given in the Appendix. The examples are most representative for common applications of the code.

- The first example is a typical slab cell problem as encountered in the analysis of fast reactor critical experiments. Its results are included in Tab. 8.1 and 8.2. Many results of similar calculations have been published in the past. A comparison of slab cell calculations using KAPER4 and MURAL of UKAEA was made in /26/.

- In the second example the new version 1.5 of KAPER4 is used for the calculation of the pin cell of a tight pitch, Pu-fuelled PWR. Calculated results for a similar cell are summarized in Tab. 8.3.

- The last example shows the use of the special version for the preparation of effective cross sections of control rods to be used for operation of a fast breeder reactor.

References

1. P.E. McGrath, E.A. Fischer

   "Calculation of Heterogeneous Fluxes, Reaction Rates
   and Reactivity Worths in the Plate Structure of Zero
   Power Fast Critical Assemblies"

   KfK 1557 (1972)
   see also: P.E. McGrath, KfK 1893 (1973)


2. D.Wintzer

   "Zur Berechnung von Heterogenitätseffekten in perio-
   dischen Zellstrukturen thermischer und schneller
   Kernreaktoren"

   KfK 743 (1969)


3. E.M. Gelbard

   "Anisotropic Neutron Diffusion in Lattices of the
   Zero-Power Plutonium Reactor Experiments"

   Nucl. Sci. Eng. 54, 327 - 340 (1974)


4. R.P. Hughes

   "A Unified Derivation of the Various Definitions of
   Lattice Cell Diffusion Coefficients"

   Nucl. Sci. Eng. 67, 85 - 90 (1978)

5. E.A. Fischer

   "Neuere Methoden zur Berechnung der anisotropen
   Neutronendiffusion in Zellgittern schneller Reak-
   toren"

   KfK 3912 (1985)


6. K.M. Case, F. de Hoffmann, G. Placzek

   "Introduction to the Theory of Neutron Diffusion",
   Vol. 1

   USAEC Report (1953)


7. B. Davison

   "Neutron Transport Theory"

   Oxford University Press, 1957


8. R. Böhme

   "Integrale Transporttheorie mit linearer Anisotropie
   der Streuung zur Berechnung der Neutronenverteilung
   in endlichen Plattenanordnungen Schneller Reaktoren"

   KfK 2501 (1977)


9. E.A. Fischer

   "Neutron Streaming in Fast Reactor Slab Lattices and
   in Cylindrical Channels"

   Nucl. Sci. Eng. 78, 227 - 238 (1981)


10. P. Benoist

    "Théorie du Coefficient de Diffusion des Neutrons dans
    un Réseau Comportant des Cavités"

    CEA-R-2278 (1964)
    see also Nucl. Sci. Eng. 34, 285 - 307 (1968)

11. IMSL Library, Problem-Solving Software System for
    Mathematical and Statistical FORTRAN Programming.
    IMSL, Inc. (1984)


12. A.P. Olson
    Mathematics of Computation, Vol. 23, 106 (1969)


13. E. Kiefhaber
    "Application of Real, Adjoint and Bilinear Weighting
    for Collapsing Group Constants Used in Space Dependent
    Neutron Diffusion Problems"

    KfK 3470 (1982),
    and H. Bachmann, R. Kiesel, D. Woll: Kurzbeschreibung
    des KAPROS-Moduls BUCITO", Internal Report (1979)


14. I. Carlvik
    "A Method for Calculating Collision Probabilities in
    General Cylindrical Geometry and Application to Flux
    Distributions and Dancoff Factors"

    Third Internat. Conf. Peaceful Uses of Atomic Energy,
    Geneva, 31 Aug. - 9 Sept. 1964
    Vol. 2, p. 225


15. A. Kavenoky
    "Calcul et Utilisation des Probabilités de Première
    Collision pour des Milieux Hétérogènes à une Dimension:
    Les Programmes ALCOLL et CORTINA"

    Note CEA-N-1077 (1969)

16. A. Sauer

    "Approximate Escape Probabilities"

    Nucl. Sci. Eng. $\underline{16}$, 329 - 335 (1963)


17. I. Gargantini, T. Pomentale

    "Rational Chebyshev Approximations to Bessel Function
    Integrals $Ki_n(x)$"

    Communications of the Association for Computing
    Machinery $\underline{7}$, 727 (1964)


18. M. Abramowitz, I.A. Stegun

    "Handbook of Mathematical Functions"

    Dover Publications, New York 1965


19. J.L. Rowlands, C.R. Eaton

    "Effective Diffusion Coefficient for Low Density
    Cylindrical Channels"

    Nucl. Sci. Eng. $\underline{76}$, 263 - 281 (1980)


20. P. Köhler, J.Ligou

    "Axial Neutron Streaming in Gas-Cooled Fast Reactors"

    Nucl. Sci. Eng. $\underline{54}$, 357 - 360 (1974)


21. J. L. Rowlands. C.R. Eaton

    "The Spatial Averaging of Cross Sections for Use in
    Transport Theory Reactor Calculations, with an Appli-
    cation to Control Rod Fine Structure Homogenisation"

    IAEA/NEA Technical Committee Meeting on Homogenisation
    Methods in Reactor Physics, Lugano, Nov. 1978
    IAEA-TECDOC-231

22. D. Woll

"GRUCAL - Ein Programmsystem zur Berechnung makroskopischer Gruppenkonstanten

KfK 2108 (1975)


23. E.A. Fischer, F. Kappler

Internal Report, March 1980
see also Ref. 26


24. G. Buckel, W. Höbel

"Das Karlsruher Programmsystem KAPROS, Teil I, Übersicht und Vereinbarungen, Einführung für Benutzer und Programmierer"

KfK 2253 (1976)

and H. Bachmann, S. Kleinheins

"Das Karlsruher Programmsystem KAPROS, Teil 1a, Kurzes KAPROS-Benutzerhandbuch"

KfK 2317 (1976)


25. D. Woll

"Aufbau der Gruppenkonstantenbibliothek GRUBA und ihre Verwaltung durch das Programmsystem GRUMA"

KfK 3745 (1984)


26. M.J. Grimstone, J.M. Stevenson, R. Böhme, E.A. Fischer

"Cell Heterogeneity Problems in the Analysis of Zero Power Experiments"

Int. Symp. Fast Reactor Physics, IAEA, Aix-en-Provence, Sept. 1979

Table 5.1: $\Delta D_z$ and $\Delta R_r$ for a Gas-Cooled Fast Breeder

$R_1$ = 0.37 cm, $R_2$ = 0.56702 cm

$\Sigma_1$   variable, $\Sigma_2$ = 2.0 x $10^{-4}$ $cm^{-1}$

| $\Sigma_1$ ($cm^{-1}$) | 0.1 | 0.2 | 0.3 | 0.4 | 0.6 | 1.0 |
|---|---|---|---|---|---|---|
| $D_{hom}$ (cm) | 7.8073 | 3.9089 | 2.6071 | 1.9558 | 1.3041 | 0.7826 |
| cylindrical cell model | | | | | | |
| $\Delta D_z$ | 0.1300 | 0.1331 | 0.1353 | 0.1371 | 0.1405 | 0.1463 |
| $\Delta D_r$ | 0.0541 | 0.0559 | 0.0572 | 0.0582 | 0.0608 | 0.0651 |
| $\frac{1}{3}(\Delta D_z + 2\Delta D_r)$ | 0.0794 | 0.0816 | 0.0832 | 0.0845 | 0.0874 | 0.0922 |
| $\Delta D_{iso}$ | 0.0792 | 0.0813 | 0.0828 | 0.0841 | 0.0866 | 0.0910 |
| Dancoff factor model | | | | | | |
| $\Delta D_z$ | 0.1578 | 0.1562 | 0.1554 | 0.1551 | 0.1556 | 0.1581 |
| $\Delta D_r$ | 0.0414 | 0.0425 | 0.0434 | 0.0443 | 0.0462 | 0.0496 |
| $\frac{1}{3}(\Delta D_z + 2\Delta D_r)$ | 0.0802 | 0.0804 | 0.0807 | 0.0812 | 0.0827 | 0.0858 |
| $\Delta D_{iso}$ | 0.0866 | 0.0863 | 0.0863 | 0.0865 | 0.0873 | 0.0896 |

Table 5.2: $D_k/D_{hom}$ for a Gas-Cooled Breeder Cell

$$\Sigma_1 = 0.59657 \ cm^{-1}, \quad \text{Variable } \Sigma_2$$

| $\Sigma_2 (cm^{-1})$ | $D_{hom}(cm)$ | $D_z/D_{hom}$ | | $D_r/D_{hom}$ | | $D_{iso}/D_{hom}$ | |
|---|---|---|---|---|---|---|---|
| | | A | B | A | B | A | B |
| 0.4 | 0.6891 | 1.0048 | 1.0063 | 1.0026 | 1.0021 | 1.0033 | 1.0036 |
| 0.2 | 0.9037 | 2.0269 | 1.0340 | 1.0142 | 1.0105 | 1.0184 | 1.0192 |
| 0.1 | 1.0703 | 1.0524 | 1.0646 | 1.0268 | 1.0197 | 1.0351 | 1.0364 |
| 0.05 | 1.1790 | 1.0723 | 1.0876 | 1.0362 | 1.0264 | 1.0479 | 1.0493 |
| 0.01 | 1.2832 | 1.1010 | 1.1133 | 1.0438 | 1.0337 | 1.0623 | 1.0636 |
| 0.0002 | 1.3116 | 1.1070 | 1.1186 | 1.0463 | 1.0351 | 1.0660 | 1.0666 |

A    Cylindrical Cell

B    with Dancoff factor

Table 6.1: Calculational model of the control rod in the supercell

1. Model dimensions and the calculational mesh (mm)

| Zone | Outer Radius | Thickness | No of Mesh Points |
|------|--------------|-----------|-------------------|
| 1 | 53.7128 | 53.7128 | 4 |
| 2 | 76.7773 | 23.0645 | 2 |
| 3 | 203.1336 | 126.3563 | 4 |

2. Atomic number densities $(10^{22}$ atoms/cm$^3)$

| Nuclide | Zone 1 | Zone 2 | Zone 3 |
|---------|--------|--------|--------|
| B10 | 1.2390 | | |
| B11 | 4.9864 | | |
| C | 1.5659 | | |
| O | | | 1.3769 |
| Na | 0.5582 | 1.5301 | 0.9407 |
| Al | | 0.0298 | |
| Si | | 0.0192 | |
| Ti | | 0.0199 | |
| V | | 0.0014 | |
| Cr | 0.1969 | 0.4399 | 0.3673 |
| Mn | 0.0179 | 0.0158 | |
| Fe | 0.7602 | 1.1536 | 1.3301 |
| Ni | 0.1270 | 0.6145 | 0.2040 |
| Cu | | 0.1547 | |
| Mo | 0.0185 | 0.0232 | |
| U235 | | | 0.0023 |
| U238 | | | 0.5698 |
| Pu239 | | | 0.0930 |
| Pu240 | | | 0.0196 |
| Pu241 | | | 0.0033 |

Table 7.1: Dimensions of KAPER4 Quantities

| quantity | symbol used | dimension in classical | : SI-units | re-mark |
|---|---|---|---|---|
| microscopic cross section | sigma,sig.. | $1b =$ $10^{-24}cm^2$ | : $1fm^2 =$ : $10^{-30}m^2$ | I |
| number density, concentration | N | $10^{24}cm^{-3}$ | : : $10^{30}m^{-3}$ | N |
| fission spectrum | CHI | 1 | : 1 | P |
| length | L,T,R | 1cm | : 1m | U |
| bucklings | $B^2$,BSQ.... | $1cm^{-2}$ | : $1m^{-2}$ | T |
| macroscopic cross section | SIGMA=sigma×N | $1cm^{-1}$ | : $1m^{-1}$ | O |
| diffusion constant | D=1/(3×SIGTR) | 1cm | : 1m | U |
| volume | V | $1cm^3$ | : $1m^3$ | T |
| adjoint | ADPHI | 1 | : 1 | P |
| flux density | PHI | $1cm^{-2}$ | : $1m^{-2}$ | U |
| reaction rate per atom | sigma×PHI | $10^{-24}$ | : $10^{-30}$ | T |
| optical thickness | SIGMA×L | 1 | : 1 | |
| leakage correction | $D×B^2$/SIGT | 1 | : 1 | |
| time | not used | 1 | : 1 | |

Table 7.2: Standard Fission Spectra in KAPER4

| Fission Spectrum | Identifying Isotope Name | Maxwellian Temperature | Associated Isotope Names |
|---|---|---|---|
| 1 | 'TH232___' | 1.32 MeV | |
| 2 | 'U 233___' | 1.31 MeV | 'NP237___' |
| 3 | 'U 234___' | 1.31 MeV | |
| 4 | 'U 235___' | 1.30 MeV | |
| 5 | 'U 236___' | 1.31 MeV | |
| 6 | 'U 238___' | 1.35 MeV | 'AM241___' |
| 7 | 'PU239___' | 1.41 MeV | 'CF252___' |
| 8 | 'PU240___' | 1.39 MeV | 'CM242___' |
| 9 | 'PU241___' | 1.34 MeV | 'PU238___','AM243___' |
| 10 | 'PU242___' | 1.39 MeV | 'CM244___' |

Note: Fröhner (1988) has suggested to use Watt's distribution instead of Maxwell's. This is not foreseen in KAPER4. As a second choice the following Maxwellian temperatures were recommended and can be used in KAPER4: 1.375 MeV for $^{239}$Pu fission ad 1.318 MeV for $^{235}$U fission (see Appendix, second case, as an example).

Table 8.1:  Plate Cell Calculations

Approach of the homogeneous limit for the plate cell of Appendix A

Isotropic diffusion

| thickness in cm | | in mfp at ≃1MeV | | $k_{eff}$ | $k_\infty$ for $k_{eff}=1$ | $k_\infty$ for $B^2=0$ | D (cm) |
|---|---|---|---|---|---|---|---|
| plate 1 | plate 2 | plate 1 | plate 2 | | | | |
| 6.2 | 5.7 | .66 | 1.65 | 0.97399 | 1.99892 | 1.79010 | 1.892 |
| .62 | .57 | .066 | .165 | 0.99677 | 1.96965 | 1.78110 | 1.756 |
| .062 | .057 | .0066 | .0165 | 1.00013 | 1.96555 | 1.77935 | 1.738 |
| .0062 | .0057 | .00066 | .00165 | 1.00045 | 1.96519 | 1.77923 | 1.737 |
| .00062 | .00057 | .000066 | .000165 | 1.00000 | 1.96490 | 1.77911 | 1.737 |
| NHOM=1 | | .000066 | .000165 | 1.00056 | 1.96520 | 1.77927 | 1.736 |
| homogenized | | .120 | .111 | 1.00055 | 1.96513 | 1.77923 | 1.736 |
| GRUCAL(χ of $^{239}$Pu)+BUCITO | | | | 0.98024 | | 1.79600 | 1.836 |

Anisotropic diffusion

| thickness in cm | | in mfp at ≃1MeV | | $k_{eff}$ | $k_\infty$ for $k_{eff}=1$ | $k_\infty$ for $B^2=0$ | D (cm) |
|---|---|---|---|---|---|---|---|
| plate 1 | plate 2 | plate 1 | plate 2 | | | | |
| 6.2 | 5.7 | .66 | 1.65 | 0.97470 | 1.99860 | 1.79010 | 1.889 |
| .62 | .57 | .066 | .165 | 0.99694 | 1.96957 | 1.78111 | 1.756 |
| .062 | .057 | .0066 | .0165 | 1.00017 | 1.96553 | 1.77935 | 1.738 |
| .0062 | .0057 | .00066 | .00165 | 1.00046 | 1.96519 | 1.77923 | 1.737 |
| .00062 | .00057 | .000066 | .000165 | 1.00000 | 1.96491 | 1.77912 | 1.737 |
| homogenized | | .120 | .111 | 1.00055 | 1.96513 | 1.77923 | 1.736 |

Notes:

26 energy groups, KFKINR cross section set; D is the diffusion coefficient calculated by collapsing $\Sigma_{tr}$ to 1 energy group; mean free path (mfp) is thickness×$\Sigma_t$ in energy group 5.

Input $B^2$: perpendicular 12.090E-4 cm$^{-2}$, parallel 21.763E-4 cm$^{-2}$.

Table 8.2:  Comparison of One Group Cross Sections

Plate cell of Appendix A,
26 energy group calculations, KFKINR cross section set.

| cell configuration: | GRUCAL homogenized | KAPER4 homogenized | KAPER4 heterogeneous |
|---|---|---|---|
| $k_\infty(B^2=0)$ | 1.7960 | 1.7792 | 1.7811 |
| $B^2(k_{eff}=1)$ | 32.48E-4 | 33.89E-4 | 33.63E-4 |
| $k_\infty(k_{eff}=1)$ | 1.9927 | 1.9654 | 1.9686 |

1-group cross sections calculated by collapsing 26 group data to one group data by application of BUCITO and COLRAB /13/:

| | | | |
|---|---|---|---|
| $\Sigma_c$ | 2.000E-3 | 2.083E-3 | 2.078E-3 |
| $\nu\Sigma_f$ | 1.197E-2 | 1.198E-2 | 1.200E-2 |
| $\Sigma_{rem}$ | 6.008E-3 | 6.096E-3 | 6.096E-3 |
| $\Sigma_f$ | 4.031E-3 | 4.035E-3 | 4.041E-3 |
| $\Sigma_{tr}$ | 0.18151 | 0.19198 | 0.18988 |

Note: $\chi$ of $^{239}$Pu used in the GRUCAL calculation;
anisotropic diffusion and recommended parameters used for the
KAPER4 calculation of the heterogeneous cell.

Table 8.3:  Comparison of KAPER4 Options

Pin cell of an advanced PWR as given in Appendix A,
69 energy groups, G69COLD cross section set.

Search for critical bucklings $B^2$, starting with $B^2 = 20.833E-4$ cm$^{-2}$.

| | recommended parameters | $\Sigma_t$ replaced by $\Sigma_{tr}$ | EPS = 1. $\Sigma_t$ replaced | GAM = 10$^4$ $\Sigma_t$ replaced | EPS < 0. $\Sigma_t$ replaced | remark |
|---|---|---|---|---|---|---|
| $k_{eff}$ | 1.03399 | 1.03393 | 1.03352 | 1.03417 | 1.03676 | $B^2$ input |
| $B^2$ | 23.380E-4 | 23.349E-4 | 23.244E-4 | 23.407E-4 | 24.042E-4 | $k_{eff}$=1 |
| $k_\infty$ | 1.10962 | 1.10957 | 1.10905 | 1.10984 | 1.11290 | $k_{eff}$=1 |

1-group cross sections calculated by collapsing 69 group data to one group
data by application of BUCITU and COLRAB /13/:

| | | | | | |
|---|---|---|---|---|---|
| $\Sigma_c$ | 1.5028E-2 | 1.5031E-2 | 1.5037E-2 | 1.5029E-2 | 1.4998E-2 |
| $\nu\Sigma_f$ | 2.6949E-2 | 2.6948E-2 | 2.6938E-2 | 2.6955E-2 | 2.7019E-2 |
| $\Sigma_{rem}$ | 2.5135E-2 | 2.5129E-2 | 2.5132E-2 | 2.5129E-2 | 2.5114E-2 |
| $\Sigma_f$ | 9.3522E-3 | 9.3519E-3 | 9.3483E-3 | 9.3544E-3 | 9.3766E-3 |
| $\Sigma_{tr}$ | 0.29254 | 0.29254 | 0.29256 | 0.29252 | 0.29246 |

Note: Recommended parameters are EPS = 0., GAM = 1000., use of $\Sigma_t$ (ITRANS=0).
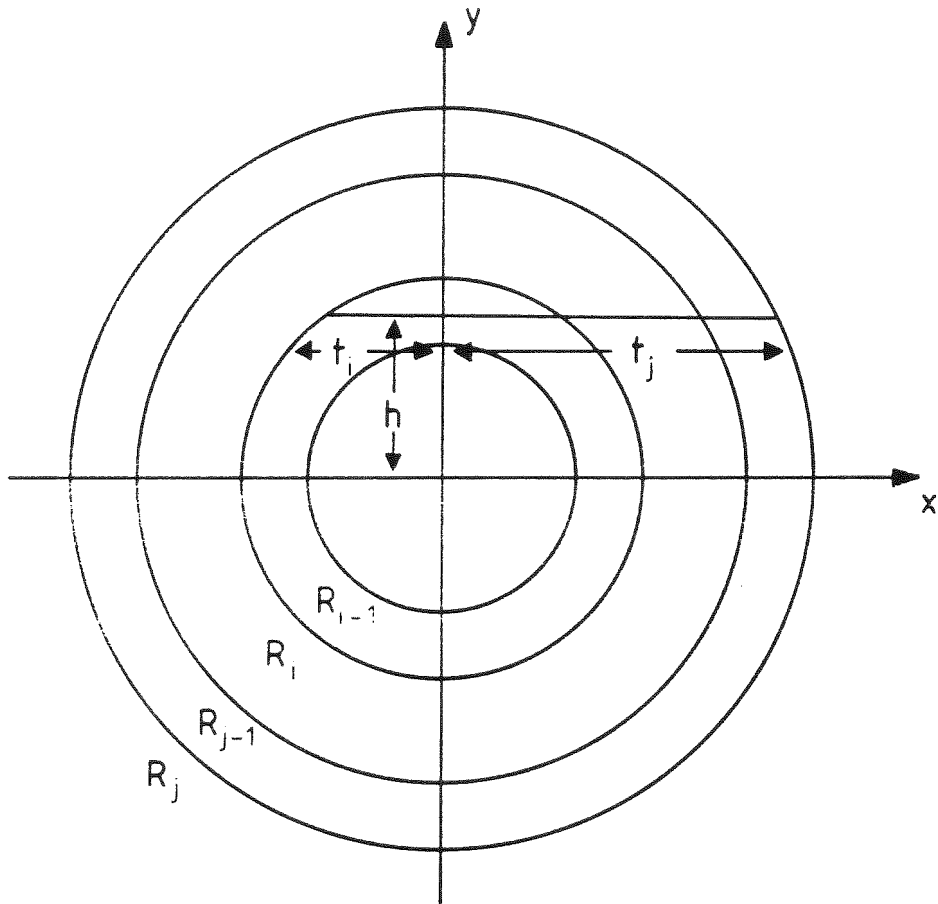
Fig.1: Regions in a Cylindrical Cell

Figure 7.1:   Geometry Options of KAPER4


KGEO=1      Plate Geometry

```
          /|       |   |         | |          |/
          /|       |   |         | |          |/
          /|       |   |         | |          |/
periodic /|← T(1) →|   |← T(i) →| |←  T(NR)  →|/ periodic
boundary /|        |   |         | |          |/ boundary
          /|       |   |         | |          |/
          /|       |   |         | |          |/
          /|       |   |         | |          |/
          /|←————————cell thickness————————→|/
```
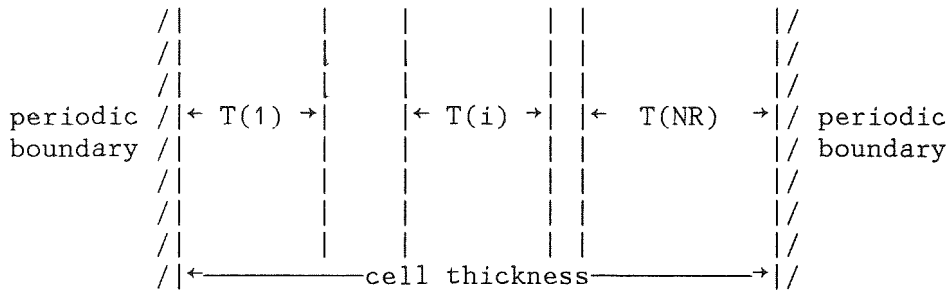

KGEO=2      Cylindrical Geometry  -circular white boundary-
            (WIGNER-SEITZ-cell)



```
              T(1)....T(NR)
```
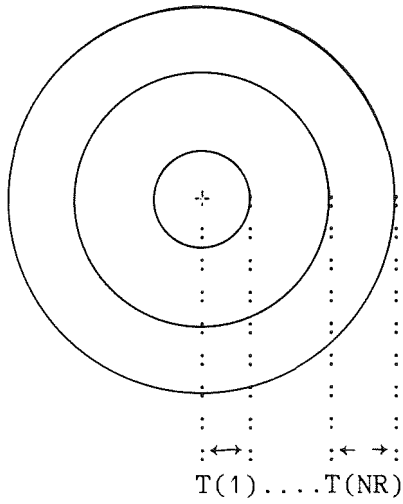

KGEO=3      Cylindrical Geometry  -square boundaries periodic-



```
              T(1)....T(NR)
```
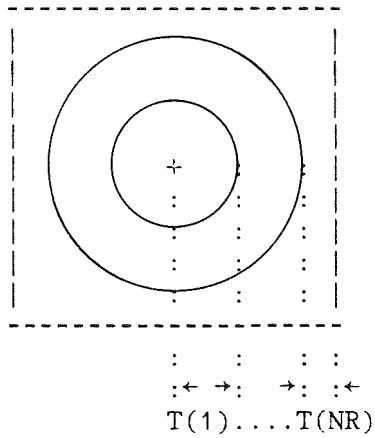
*Figure 7.1 continued*

KGEO=4　　Cylindrical Geometry　-hexagonal boundaries periodic-
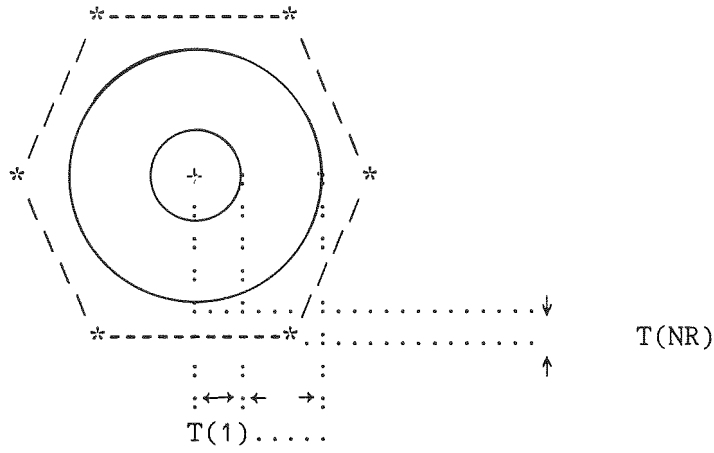
Figure 7.2: Definition of Directions

a) Plate Geometry (KGEO=1)



parallel (BSQPARA)
infinite extension

perpendicular
(BSQPERP)
infinite repetition

← T(1) →     ← T(i) →     ← T(NR) →

←————————cell thickness————————→
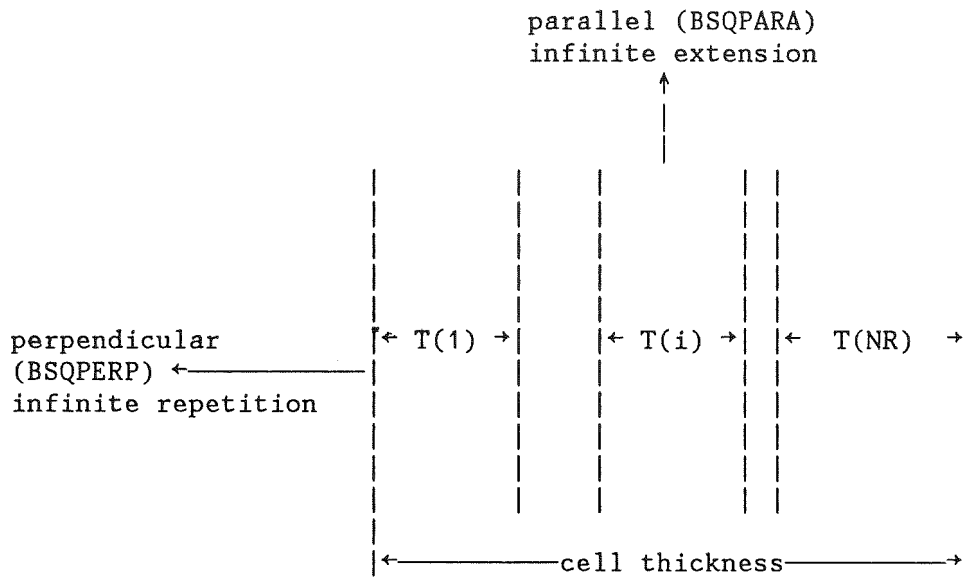
b) Cylindrical Geometry (KGEO > 1)



parallel (BSQPARA)
infinite extension

perpendicular
(BSQPERP)
infinite repetition
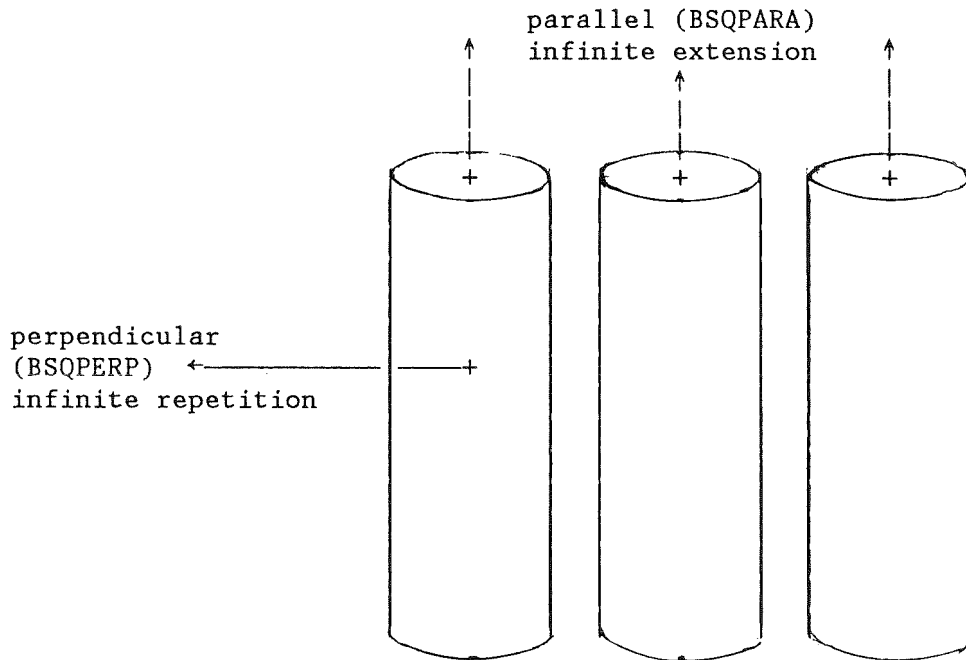
APPENDIX : Input Examples of KAPER4, Version 1.5

1)   TWO REGION PLATE CELL

        1ST STEP: CROSS SECTION PREPARATION FOR NORMAL PLATE CELL
        2ND STEP: CROSS SECTION PREPARATION FOR PERTURBED CELL
        3RD STEP: CROSS SECTION PREPARATION FOR PERTURBATION SAMPLE
        4TH STEP: CROSS SECTION PREPARATION FOR HOMOG. PERTURBATION SAMPLE
        5TH STEP: FLUX CALCULATION, EIGEN VALUE PROBLEM AND BOUNDARY SOURCE
                  PROBLEM
        6TH STEP: PERTURBATION CALCULATION

```
//JOBCARD
//*
// EXEC KSCLG7
//*          DA-UNIT CONTAINING MICROSCOPIC CROSS SECTIONS
//K.FT01F001 DD DISP=SHR,DSN=...........KFKINR
//*          UNIT FOR ADDITIONAL OUTPUT, FORMATED
//K.FT10F001 DD UNIT=DISK,DISP=(,CATLG),SPACE=(TRK,(3,1),RLSE),
//   VOL=SER=BAT00C,DSN=.......KAPER.DATA,
//   DCB=(LRECL=80,BLKSIZE=3120,RECFM=FB)
//*          UNITS FOR DATA TRANSFER, UNFORMATED
//K.FT15F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(TRK,(9,9)),DCB=DCB.VBS
//K.FT16F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(TRK,(9,9)),DCB=DCB.VBS
//K.FT17F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(TRK,(9,9)),DCB=DCB.VBS
//K.FT18F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(CYL,(1,5)),DCB=DCB.VBS
//K.FT19F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(CYL,(1,5)),DCB=DCB.VBS
//K.SYSIN DD *
*KSIOX DBN=KAPER INPUT,IND=1,PMN=PRKAP4,TYP=CARD
*$
*$ STEP 1 INPUT PHASE SSXS
*$
*$ K1 :'SSXS'
       'SSXS'
*$ K2 : GRSN
       'KFKINR  '
*$ K3 : NOG   NB  KGEO   IHI   NOR  NCHI  ITRANS
        26    6    1     10     0    0      0
*$ K4 : GAM    EPS
       1000.   0.
*$ K5 : NIS,  (ISOT(I),TEMPT(I),I=1,NIS)
           6
'PU239  ' 300. 'U 238  ' 300. 'PU240  ' 900. 'O       ' 900.
'NA      ' 900. 'FE      ' 900.
*$ K6 : NISS, IF(NISS.GT.0):(ISON(I),I=1,NISS)
           1                 'FE      '
*$ K7 : NR,  (T(I),I=1,NR),   (MIX(I),I=1,NR)
         2   0.62   0.57        1 2
*$ K8 : NMIX,((CON(J,I),I=1,NIS),J=1,NMIX)
2
*$ MIXTURE 1
 1.0-8     0.0       0.0       0.0       1.7-2     1.5-2
*$ MIXTURE 2
 4.3-3     1.2-2     4.-4      3.3-2     0.0       1.5-2
*$ K9 : MPERT, NAP,  IF(NOR.GT.0):(IS(I),I=1,NOR)
          0   -15
*$ K10 TO K14 : CHI,TEMP,ETC. SEE KAPROS NOTE 64      --- IF NCHI.NE.0
```

```
*$
*$ STEP 2 INPUT PHASE SSXS
*$
        'SSXS'
        'KFKINR '
        26    6     1     0     0     0     0
        1000.    0.
              6
'PU239   '  900.  'U 238   '  900.  'PU240   '  900.  'O       '  900.
'NA      '  900.  'FE      '  900.
              1                      'FE       '
        2   0.31   0.235      1 2
2
 1.0-8     0.0       0.0       0.0       1.7-2     1.5-2
 4.3-3     1.2-2     4.-4      3.3-2     0.0       1.5-2
        1  -16
*$
*$ STEP 3 INPUT PHASE SSXS
*$
        'SSXS'
        'KFKINR '
        26    6     1     0     0     0     0
        1000.    0.
              6
'PU239   '  900.  'U 238   '  900.  'PU240   '  900.  'O       '  900.
'NA      '  900.  'FE      '  900.
              1                      'FE       '
        2   0.31   0.235      1 3
3
 1.0-8     0.0       0.0       0.0       1.7-2     1.5-2
 4.3-3     1.2-2     4.-4      3.3-2     0.0       1.5-2
 .1854127-2 .5174309-2 .1724771-3 .1422936-1 .9669717-2 .1499999-1
        1  -17
*$
*$ STEP 4 INPUT PHASE SSXS
*$
        'SSXS'
        'KFKINR '
        26    6    -1     0     0     0     0
        1000.    0.
              6
'PU239   '  900.  'U 238   '  900.  'PU240   '  900.  'O       '  900.
'NA      '  900.  'FE      '  900.
              1                      'FE       '
        2   0.31   0.235      1 3
3
 1.0-8     0.0       0.0       0.0       1.7-2     1.5-2
 4.3-3     1.2-2     4.-4      3.3-2     0.0       1.5-2
 .1854127-2 .5174309-2 .1724771-3 .1422936-1 .9669717-2 .1499999-1
        1   17
*$
*$ STEP 5 INPUT PHASE FLUX
*$
*$ K1: 'FLUX'
        'FLUX'
*$ K2: NHOM  NXST NPERT    IB KBSQ  NGC   IAN  IHCS
         0    15    16     26   0    0     1     0
```

```
*$ K3: IMIN   IMAX  EPSPHI    EPSKEF
          4    20    1.-5      1.-5
*$ K5B: (BSQPARA(K),K=1,NOG),(BSQPERP(K),K=1,NOG)    --- IB>1,IAN>0
  0.6181E-02  0.6192E-02  0.5629E-02  0.5214E-02  0.4682E-02  0.3195E-02
  0.2250E-02  0.7545E-03  0.1283E-03  0.9598E-04 -0.5251E-03 -0.9357E-03
 -0.1429E-02 -0.5181E-02 -0.6483E-02 -0.1005E-01 -0.1516E-01 -0.2757E-01
 -0.2301E-01 -0.2061E-01 -0.1085E-01 -0.8730E-02 -0.2038E-01 -0.9632E-02
 -0.6883E-02 -0.6354E-02
                          0.5136E-03  0.5135E-03  0.5226E-03  0.5307E-03
  0.5433E-03  0.6031E-03  0.6842E-03  0.1069E-02  0.1250E-02  0.9464E-03
  0.6930E-03  0.6386E-03  0.5986E-03  0.5007E-03  0.4890E-03  0.4706E-03
  0.4581E-03  0.4461E-03  0.4491E-03  0.4512E-03  0.4680E-03  0.4759E-03
  0.4514E-03  0.4722E-03  0.4861E-03  0.4900E-03
*$
*$ STEP 6 INPUT PHASE PERT
*$
*$ K1: 'PERT'
       'PERT'
*$ K2:  NFLUX  NPERT  NXECT  NTAPE  NTAPE1  NSAM   NFP    NCELL
          15     16     17     18      19     2      3      +3
*$ K3:   IH     IH1    MORE   NUNPER
          0      1      -1      0
*$ K4:  ENORM
          1.
*$ K5:  (VOID(I),I=1,NW)                         --- IF MORE=-1
         0.5 0.5
*$ K6:  NT (TITLE(I),I=1,NT)                     --- REPEAT NSAM TIMES
         2  'TEST1111'
         3  'TEST22222222'
*$
*$ END OF INPUT PHASE PERT
*$
*$*$
*GO SM=KAPER4,MPARM=1
/*
//
```

2)   PIN CELL OF AN ADVANCED PWR LATTICE (SOME DATA ALTERED)

     1ST STEP: CROSS SECTION PREPARATION FOR PIN CELL
     2ND STEP: FLUX CALCULATION, EIGEN VALUE PROBLEM AND REACTION RATES

```
//JOBCARD
//*
// EXEC KSCLG7
//*         DA-UNIT CONTAINING MICROSCOPIC CROSS SECTIONS
//K.FT01F001 DD DISP=SHR,DSN=...........G69COLD,LABEL=(,,,IN)
//*         UNIT FOR STORAGE OF KAPER4 GROUP CONSTANTS
//K.FT15F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(TRK,(10,5),RLSE),
// DCB=(RECFM=VBS,BLKSIZE=16376),DSN=&SSXS
//K.SYSIN DD *
```

```
*KSIOX DBN=KAPER INPUT,IND=1,PMN=PRKAP4,TYP=CARD
*$
*$ K1 :'SSXS'
        'SSXS'
*$ K2 : GRSN
        'WIMSLIB '
*$ K3 : NOG   NB  KGEO   IHI    NOR   NCHI   ITRANS
         69   6     4     6      8     -8     -100
*$ K4 : GAM      EPS
        1000.    0.
*$ K5 : NIS,   (ISOT(I),TEMPT(I),I=1,NIS)
20
'U 235   ' 300. 'U 238   ' 300. 'PU238   ' 900. 'PU239   ' 300.
'PU240   ' 900. 'PU241   ' 900. 'PU242   ' 900. 'AM241   ' 900.
'FE      ' 300. 'CR      ' 300. 'NI      ' 300. 'MO      ' 300.
'MN      ' 300. 'SI      ' 300. 'CU      ' 300. 'AL      ' 300.
'HE  4   ' 300. 'H       ' 300. 'C       ' 300. 'O       ' 300.
*$ K6 : NISS, IF(NISS.GT.0):(ISON(I),I=1,NISS)
        1 'H             '
*$ K7 : NR,   (D(I),I=1,NR),   (MIS(I),I=1,NR)
     3          .423 .0557 .0563        1 2 3 *$ HEXAGONAL, KGEO=4
*$ K8 : NMIX,((CON(J,I),I=1,NIS),J=1,NMIX)
3
*$ MIXTURE FUEL
1.-4      2.-2      2.-5      1.5-3     5.-4      1.-4      1.-4      1.-5
3.-5      0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 4.6-2
*$ MIXTURE 2 CLAD STEEL AIR
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
4.8-2    1.-2      9.-3      1.-3      6.-4      8.-4      2.-4      4.-6
4.-6      0.000000 9.-5      0.000000
*$ MIXTURE 3 MODERATOR H2O
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 6.6-2    0.000000 3.3-2
*$ K9 : MPERT, NAP,  IF(NOR.GT.0):(IS(I),I=1,NOR)
            0   -15    1 2 3 4 5 6 7 8
*$ K12: NI, NE
        2   +1
*$ K13: N, (E(K),K=1,N)                         --- IF NE>0
        69   *$ ENERGY LIMITS IN MEV
10.0000        6.06550       3.67900       2.23100       1.35300
  .821000       .500000       .302500       .183000       .111000
  .673400E-01   .408500E-01   .247800E-01   .150300E-01   .911800E-02
  .553000E-02   .351910E-02   .223945E-02   .142510E-02   .906898E-03
  .367262E-03   .148728E-03   .755014E-04   .480520E-04   .277000E-04
  .159680E-04   .987700E-05   .400000E-05   .330000E-05   .260000E-05
  .210000E-05   .150000E-05   .130000E-05   .115000E-05   .112300E-05
  .109700E-05   .107100E-05   .104500E-05   .102000E-05   .996000E-06
  .972000E-06   .950000E-06   .910000E-06   .850000E-06   .780000E-06
  .625000E-06   .500000E-06   .400000E-06   .350000E-06   .320000E-06
  .300000E-06   .280000E-06   .250000E-06   .220000E-06   .180000E-06
  .140000E-06   .100000E-06   .800000E-07   .670000E-07   .580000E-07
  .500000E-07   .420000E-07   .350000E-07   .300000E-07   .250000E-07
  .200000E-07   .150000E-07   .100000E-07   .500000E-08
*$ K14: NAME, TEMP                              --- IF NI>0
   'U 235   ' 1.318  *$ NEW MAXWELL TEMPERATURES 1988
```

```
      'PU239    ' 1.375  *$ NEW MAXWELL TEMPERATURES 1988
*$
*$ STEP 2 INPUT PHASE FLUX
*$
*$ K1: 'FLUX'
       'FLUX'
*$ K2: NHOM  NXST NPERT   IB KBSQ  NGC   IAN  IHCS
         0   -15    0    69   1     0     0    -1
*$ K3: IMIN  IMAX EPSPHI   EPSKEF
         4    20   1.-5     1.-5
*$ K5A:(BSQ(K),K=1,NOG)                        --- IB>1,IAN=0
      69*20.-4
*$ K6: MAXB   AKE    EBK    FAK   NBQ          --- IF(KBSQ.NE.0)
         5    1.    5.-5    0.    0.
*$ K7A:  FAKMAK FAKMIK FAKCHI FAKD  IPRINT(0 NOPRINT)-- IF(IHCS.LT.0)
         4*1.                         0
*$ K7B:  IM    IRR  IZ  MSIG  MCHI   IS  IE    --- IF(IHCS.NE.0)
         1     8    0    0     0     -1   3
*$ K7A:  FAKMAK FAKMIK FAKCHI FAKD  IPRINT(0 NOPRINT)-- IF(IHCS.LT.0)
         4*1.                         1
*$ K7B:  IM    IRR  IZ  MSIG  MCHI   IS  IE    --- IF(IHCS.NE.0)
        -1    -8    0    0     0     1    3
*$ K8:  (TYPE(I),I=1,IZ)                       --- IF (IZ.GT.0)
*$ K9:   NG   (NEWG(I),I=1,NG)                 --- IF (IM.LT.0)
          1     1
*$ K10: NUT  NUK   (NRR(I),I=1,NUK)            --- IF(IRR.LT.0)
          6   1    1
*$
*$ END OF INPUT PHASE FLUX                     --- IF PRECEDING IS.GE.0
*$*$
*GO SM=KAPER4
//
```

3)   CROSS SECTIONS OF A SINGULARITY IN CYLINDRICAL GEOMETRY
     (ABSORBER SUPERCELL OF A LMFBR HOMOGENIZED)

```
//JOBCARD
//**
// EXEC KSCLG7
//*          DA-UNIT CONTAINING MICROSCOPIC CROSS SECTIONS
//K.FT01F001 DD DISP=SHR,DSN=...........KFKINR
//*          UNIT FOR STORAGE OF KAPER4 GROUP CONSTANTS
//K.FT15F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(TRK,(9,9)),DCB=DCB.VBS
//K.SYSIN DD *
*KSIOX DBN=KAPER INPUT,IND=1,PMN=PRKAP4,TYP=CARD
*$
*$ STEP 1 INPUT PHASE SSXS
*$
*$ K1 :'SSXS'
       'SSXS'
*$ K2 : GRSN
       'KFKINR  '
*$ K3 : NOG   NB  KGEO   IHI   NOR  NCHI  ITRANS
         26    6    2     6     3    0      0
```

```
*$ K4 : GAM      EPS
        1000.    0.
*$
*$ K5 : NIS,   (ISOT(I),TEMPT(I),I=1,NIS)
  16
'PU239   ' 900.  'PU240   ' 900.  'PU241   ' 900.  'PU242   ' 900.
'U 235   ' 900.  'U 238   ' 900.  'O       ' 900.  'NA      ' 900.
'MO      ' 900.  'NI      ' 900.  'NB      ' 900.  'FE      ' 900.
'CR      ' 900.  'B 10    ' 900.  'B 11    ' 900.  'C       ' 900.
*$ K6 : NISS, IF(NISS.GT.0):(ISON(I),I=1,NISS)
         0
*$ K7 : NR,  (D(I),I=1,NR),  (MIS(I),I=1,NR)
         2    6.0     8.0     1 2
*$ K8 : NMIX,((CON(J,I),I=1,NIS),J=1,NMIX)
         2
*$ MIXTURE 1
7*0.         1.-2        0.2-3       0.4-2       0.3-4       0.2-1
0.5-2        0.9-2       1.-2        0.5-2
*$ MIXTURE 2
0.1-2        0.3-3       0.4-4       0.2-4       0.3-4       0.4-2
0.1-1        0.1-1       0.1-3       0.2-2       0.3-4       0.1-1
0.3-2        0.          0.          0.
*$ K9 : MPERT, NAP,   IF(NOR.GT.0):(IS(I),I=1,NOR)
          0   -15                    1 5 6
*$
*$ STEP 2 INPUT PHASE FLUX
*$
*$ K1: 'FLUX'
       'FLUX'
*$ K2: NHOM  NXST NPERT    IB  KBSQ  NGC    IAN   IHCS
*$      IHCS = NR -1 CAUSES CALCULATION OF A SINGULARITY
          0   -15     0    26    0    0     1     1
*$ K3: IMIN   IMAX  EPSPHI    EPSKEF
          4     20    1.-5      1.-5
*$ K5B: (BSQPARA(K),K=1,NOG),(BSQPERP(K),K=1,NOG)   ---  IB>1,IAN>0
        7.52-4  7.40-4 7.41-4  7.50-4  7.67-4  7.84-4
        7.94-4  7.66-4 7.66-4  8.38-4  8.63-4  12.0-4
        14.0-4  16.7-4 19.6-4  22.5-4  25.7-4  29.4-4
        30.0-4  32.7-4 26.9-4 -44.7-4 -53.9-4 -29.3-4
        17.0-4  31.5-4
        26*0.
*$ K7B:  IM    IRR  IZ  MSIG  MCHI    IS   IE       ---  IF(IHCS.NE.0)
          1    -3   2    0     0      1    1
*$ K8:  (TYPE(I),I=1,IZ)                             ---  IF (IZ.GT.0)
        'PE' 'FV'
*$ K10: NUT  NUK    (NRR(I),I=1,NUK)                 ---  IF(IRR.LT.0)
          6    2     1 2
*$*$
*GO SM=KAPER4
//
```