

Homogenisation Problems in Thermal and Fast Reactors

compiled by  
H.Küsters

1. Introduction

In this report we discuss some problems, which arise in connection with special space- and energy-representations in the calculational procedures for thermal and fast reactor core configurations. Following topics are investigated:

- a) The influence of the grain structure in HTR-fuel.
- b) Heterogeneity effects arising in fast-thermal test loops.
- c) Lattice-calculations in fast zero power reactors.
- d) Resonance phenomena near interfaces and boundaries in fast systems.

2. The Influence of the grain structure in HTR-Fuel

The coated particles of HTR-pebble-bed reactor fuel contain high enriched Uranium grains inbedded in graphite. The presence of graphite in the "fuel zone" has to include the elastic scattering of neutrons with graphite in the calculation of the effective resonance integral. Teuchert /1/ developed a method to calculate the resonance integral for the situation of a double heterogeneous structure in pebble bed cores. In this method the first flight of a neutron through the zones of a coated particle or a fuel sphere is calculated exactly. The geometrical escape probability  $P(\sigma_a)$  is composed by four components. In Fig. 1 we have shown the location of one coated particle in the graphite matrix. The notation is as follows:

- L : average distance between coated particles
- $\Sigma_1$  : macroscopic cross section of inner zone of coated particle
- $\Sigma_2$  : macroscopic cross section of coating
- $\alpha\Sigma_2$  : macroscopic cross section of graphite

- r : Radius  
l<sub>n</sub> : cord lengths  
dr : volume element  
v : angle, characterizing the direction of neutron flightpath  
w<sub>1</sub> is the probability for a neutron which starts in the inner zone of a coated particle, has its next collision in the coating zone of the same particle  
w<sub>2</sub> is the probability that the neutron leaves the coated particle without any collision.  
w<sub>3</sub> is the probability that a neutron, which has left a coated particle, has its next collision in the coating zone of any other coated particle within the same sphere.  
w<sub>4</sub> is the probability that the neutron leaves the sphere.

Then the escape probability is given by

$$P(\sigma_a) = w_1 + w_2(w_3 + w_4)$$

According to this procedure the effective resonance integrals can be calculated, using the formalism of Nordheim and Kuncir /2/. Important differences were obtained compared to the case where no "internal" heterogeneity has been considered.

To have an experimental check on the theoretical model, experiments have been performed with the lead slowing down spectrometer for HTR fuel containing thorium /3/.

In Fig. 2 measured and calculated resonance integrals are compared. Both the upper curves are calculations and experiments for homogeneous mixture, of ThO<sub>2</sub> kernels with graphite. The values of the theoretical predictions are a bit too high. A decrease of nearly a factor of two is observed compared to this homogeneous distributions, if coated particles are used. Theory agrees satisfactorily with experiment.

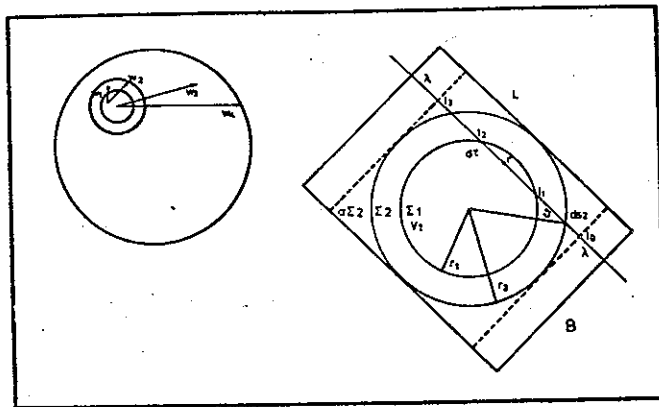


Fig. 1: Geometrical Representation of Coated Particles in a fuel sphere

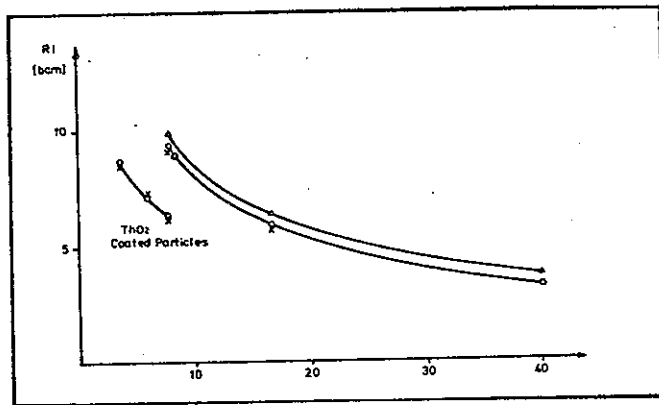


Fig. 2: Resonance integral

3. Investigation of Heterogeneity Effects arising in Fast-Thermal Test Loops. (H. Borgwaldt, J. Lolich, GfK)

A series of irradiation experiments and calculations is under way in order to assess the heterogeneity effects which may occur in the MOL 7C experiments. The irradiation experiments are performed, on bundles of highly enriched fuel rods, in the 10 cm diameter channel of the central graphite blanket of the Argonaut reactor ARK. Configuration A in the table below, consisted of a central rod and 12 outer rods on a ring of 1.64 cm radius. The rod diameter was 6.9 mm, the U-235 enrichment 20 percent, the rest of the channel was empty (air). For some calculations this true configuration was also transformed into a simplified configuration B, which treats the outer ring of rods as a homogenized ring zone with a suitably reduced smear density. This simplified configuration B was needed for calculations with the RABBLE code /4/. The WIMS code /5/ and the Monte Carlo code KAMCCO /6/ can treat both configurations.

The quantities measured and calculated were:

- $R_1$  ratio of the U-235 fission rate densities in the central and the outer rods of the bundle,
- $R_2$  the same ratio for an inner disc and an outer ring zone of the central rod,
- $R_3$  the same ratio for an inner disc and an outer ring zone of an outer rod.

In the table below, one should note the difference between the true configuration A and the simplified B and the large deviation of the RABBLE  $R_1$  value from experimental and Monte Carlo results. This large deviation led us to make additional calculations and experiments in order to check the reliability of the methods in use.

Firstly, free parameters in the RABBLE code, which determine, e.g., the spatial and energy grids, were changed on a wide scale but without any significant influence.

Secondly, we tested the influence of an assumption made in the RABBLE code, viz. that all partial currents  $J^+$ ,  $J^-$  across region boundaries have a cosine angular distribution. For this purpose we introduced a test modification

into the Monte Carlo code KAMCCO, enforcing the same cosine distribution on all neutrons crossing region boundaries.

The result for  $R_1$ , obtained in a 20 minutes run, is included in row 6 in the table. It shows an effect, which is far too small to explain the deviation of RABBLE by this assumed angular distribution.

Thirdly, additional results have been obtained from the WIMS code, rows 2 and 4 of the table, which agree rather well with the experiment and KAMCCO computations (these do not use identical nuclear Data). This applies also to the difference between the configurations A and B.

Our conclusion, at this stage, is that the experimental method can be trusted and that the available version of the RABBLE code and/or data can, for unexplained reasons, not be reliably applied.

In addition to this first set-up, a number of rod bundle irradiation experiments with hexagonal and square arrays have been performed, their degree of complication approaches MOL 7C more closely. Without going into the numerical results, which will be reported in due detail elsewhere, we want to mention that, quite generally, the agreement between experiments and calculations with WIMS and/or KAMCCO is satisfactory. It seems advantageous, considering performance and computer costs, to use WIMS for standard calculations and apply KAMCCO selectively, especially for the computation of some important details, which are not covered by the simple geometrical options and the physics model implemented in WIMS.

Comparison of Results

Method	Configuration	$R_1$	$R_2$	$R_3$
Experiment	A	.95 ± 3 %	.95 ± 2 %	.94 ± 2 %
WIMS	A	.96	.95	.97
KAMCCO	A	.94 ± 2.0 %	.93 ± 2.0 %	.95 ± .6 %
WIMS	B	.93	.95	X
KAMCCO	B	.90 ± 2.0 %	.93 ± 2.0 %	
modified KAMCCO	B	.88 ± 1.8 %	-	
RABBLE	B	.81	.95	

#### 4. Lattice-Calculations in Fast Zero Power Reactors

This section is taken from general review on fast reactor physics work /7/.

The KAPER program /8/ is a multigroup lattice code developed to analyze experiments performed in plate-type heterogeneous critical facilities. These experiments include those in which the flux fine structure in the lattice must be taken into account, as for example reaction rate and small sample reactivity worth measurements.

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

The fundamental basis of the program is integral transport theory in the collision probability formulation. The multigroup resonance self-shielded cross sections for the multiregion cell are defined by a procedure utilizing the concept of the composition-dependent self-shielding factor ("f-factor") for a homogeneous medium. A consistent formulation for the heterogeneous medium was developed through the integration of the energy and space dependent integral transport equation. The method in KAPER represents an improvement in the method originally developed by Wintzer for his ZERA code /9/. Despite the fact that the f-factor concept represents an approximation in that it contains no information on the distribution of the resonances of one particular isotope within an energy group, the experience has been that the accuracy and utility of the method for routine calculations is more than satisfactory.

The essential difference between the KAPER and ZERA codes lies in the fact that in KAPER the Boltzmann equation is solved in terms of the neutron flux, rather than the neutron source densities as done in ZERA. It must be emphasized that formally both concepts are equivalent within the narrow resonance approximation. However, it could be shown that the "flux equations" and the use of effective cross sections in KAPER (with the source density as a weighting function) yields more accurate results than the "source-

density equations" and the use of reaction coefficients in ZERA. The reason is a relatively strong dependence of the reaction coefficients on the background cross section used in the f-factor concept. This is not the case in the consistent KAPER approach, where in addition the effective cross section are only weakly dependent on the source density weighting function.

The program KAPER has a particular feature which allows one to calculate the flux distributions (real and adjoint) and reaction rates in a cell differing from the normal cells of the core. This feature has great utility for analyzing experiments that disturb the properties of the cell in the measurement procedure. For example, a cell or 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 in the position in which a sample is to be placed. In both of these cases the periodicity of the cell is disturbed. To solve for the flux it is assumed that at some point removed from the disturbance the equilibrium spectrum of the normal core cell is reestablished. The equilibrium spectrum acts as an external source for the region of disturbance. Therefore the integral transport equation is solved in this region as a fixed source equation. This procedure was checked through a series of reaction rate measurements with thin foils between varying thicknesses of aluminum and stainless steel. The experimental results were well reproduced by the KAPER program. Included in the KAPER program is a procedure to account for anisotropic diffusion of neutrons. In some experiments, such as sodium void measurements, this may be an important effect which results from the orientation of the plates in the facility. The components of the neutron diffusion, parallel and perpendicular to the plates, are calculated in the heterogeneous cell by utilizing the mean square distance between the collisions of the neutron in an energy group. The procedure is equivalent to the work of Benoist if one neglects the angular correlation terms. The procedure proved quite adequate for the analysis of an axial sodium void traverse experiment performed in the SNEAK fast critical assembly in which the plate orientation was rotated  $90^\circ$  between two experiments.

Reactivity worths are calculated with an exact perturbation formulation of the integral transport equation. By exact is meant that the perturbed

flux and unperturbed adjoint are used in the formulation. The perturbed flux in the sample and sample environment is found by the same procedure utilized for the calculation of the flux in a cell different than the normal core cell as explained above.

The experience has been that the consistency of the calculated reactivity worth results improves by several percent, depending on the sample size and the core spectrum, over the results of the normally used first order homogeneous perturbation theory.

Contrary to almost all operating computer codes the KAPER program utilizes for each fissionable isotope its own fission neutron spectrum. This feature is found to be quite important in the calculation of reactivity worths; for example the calculations of the worth of a  $^{235}\text{U}$  sample in a mixed oxide core where the major fission neutron contribution is from Pu. In this case the  $^{235}\text{U}$  worth can vary by several percent depending on whether an average core fission spectrum, from Pu, is used or the fission spectrum for each individual fissionable isotope. To demonstrate the improvement in KAPER over ZERA,  $k_{\infty}$  was calculated for a cell similar to SNEAK-5C /10/. This was a null-reactivity assembly with a soft spectrum and strong heterogeneity effects, which contained mainly mixed oxide and graphite.

The table shows the  $k_{\infty}$  values obtained for cells of different thickness. The following comments can be made:

- a) As expected from the theory, all results for the quasihomogeneous case agree well. This indicates that no programming errors are involved.
- b) The two codes, ZERA and KAPER, using the same approximation for the collision probabilities, give  $k$  values which differ by 0.6 % for the full cell, and less than that for the smaller cells. Thus, the standard ZERA code may be used unless large heterogeneities are involved.
- c) The  $k_{\infty}$  values before iteration on the source densities are given in brackets. The figures indicate that the changes due to the iteration are by one order of magnitude smaller than the difference in values given by the two codes. Therefore the iteration is necessary only in cases of large heterogeneity.



$k_{\infty}$  for the SNEAK-5C Simplified Cell

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

<sup>+</sup>)  $k_{\infty}$  values in parantheses are values before iteration on the source densities

## 5. Resonance Phenomena near Interfaces and Boundaries in Fast Systems

This section is taken from a general review on fast reactor physics /7/.

In the f-factor formalism boundary effects of resonance self shielding are not taken into account. The space dependence of the resonance self shielding is caused by the resonance structure of the neutron flux. Within a homogeneous mixture, far from boundaries, this resonance structure is fairly independent of position. Across interfaces the resonance structure of the neutron flux is influenced by the cross sections of the media on both sides of the interface and is rapidly varying with space. For the case of two adjacent half spaces, assuming NR-approximation, a solution for the neutron flux from the integral Boltzmann-equation for isotropic scattering can be given within a resonance. This solution is used as weighting function for the effective space dependent group cross sections. These in principle can be calculated directly from the resonance cross sections. But this direct calculation must be done for every combination of isotopes on both sides of an interface and would be very time consuming.

With the help of a rational approximation of the exponential integral

$$1 - E_2(x) = \frac{1,260578 \cdot x}{0,363948 + x} - \frac{0,260578 x}{2,60162 + x}$$

an approximate calculation of the space dependent effective group cross section from f-factor tables is possible /11/. The f-factors are tabulated as a function of a background cross section  $\sigma_0$ . The rational approximation allows a transformation of the space dependence to a  $\sigma_0$ -dependence. Two terms for the rational approximation turned out to be sufficient. The formalism has also been extended to thin zones.

Following remarks can be made:

The space dependent resonance self shielding is only important within two mean free paths on both sides of interfaces.

For small reflected systems, space dependent resonance self shielding leads to higher elastic scattering rates in the reflector. The consequence of this is normally a higher criticality.

At the core-blanket interface of fast reactors effects of space dependent resonance self shielding must be expected because of the higher  $^{238}\text{U}$  concentration in the blanket than in the core. In the blanket the absorption rate will be higher by several percents than predicted with space independent group cross sections. This means that the Pu production is changed. For power reactors this can cause local changes of the power distribution at the interface of several percent, because more  $^{239}\text{Pu}$  is produced. In the following figure an example for the change of the absorption rates in  $^{238}\text{U}$  for the fast critical assembly SNEAK-3A2 /12/ is given.

#### 6. Further Improvements in the Treatment of Interfaces

For the interpretation of fast zero power experiments near zones of different absorbing media, e.g. the core/blanket interface, the methods outlined in section 5 is not applicable because of the lattice character of the experiment. Therefore the KAPER-code for an infinite lattice was improved /13/ by taking into account additionally

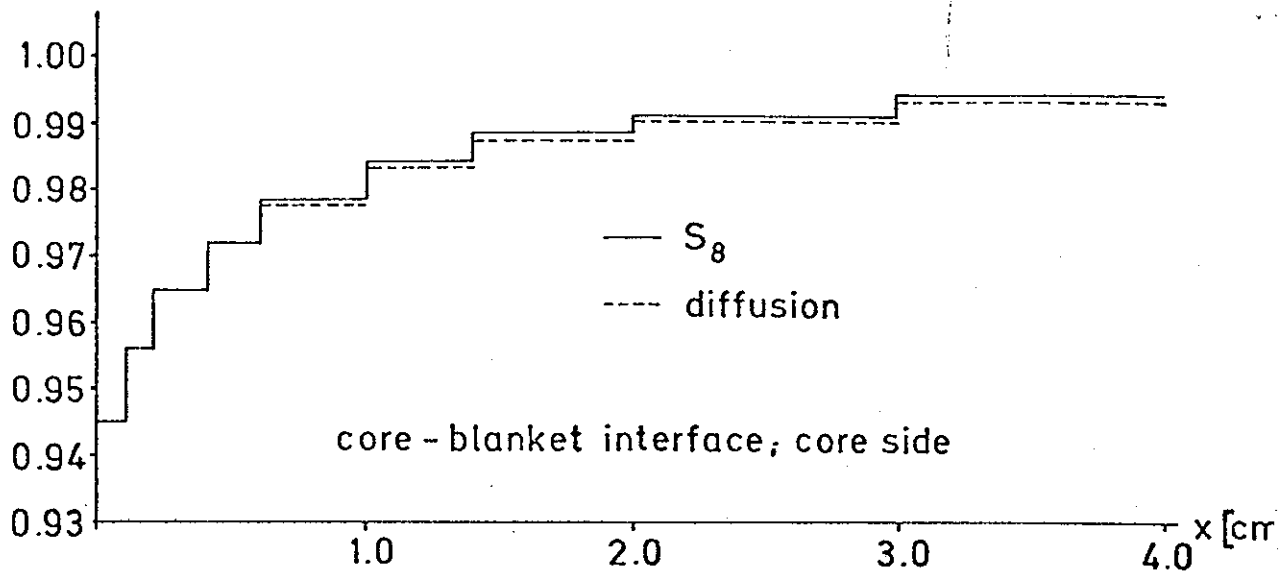
- a) the space dependence of the source density,
- b) anisotropic elastic scattering.

Thus the new code is capable to describe the true physical effects near an interface. First results show an excellent agreement with experiment.

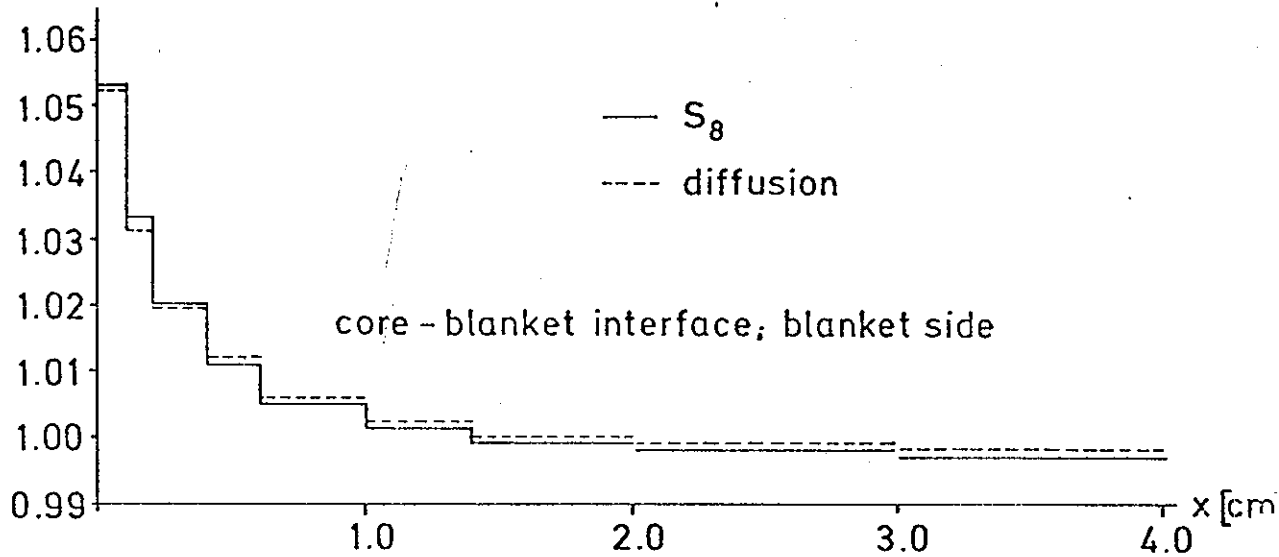
#### 7. Conclusion

By the methods outlined in this review, the theoretical tools are capable to treat satisfactorily well the heterogeneous structure of HTR-fuel and LMFBR lattices. The problem of control rods and control rod-followers is discussed elsewhere. From this it is concluded that in principle no major uncertainties arise for the question of homogenisation for whole core reactor calculations.

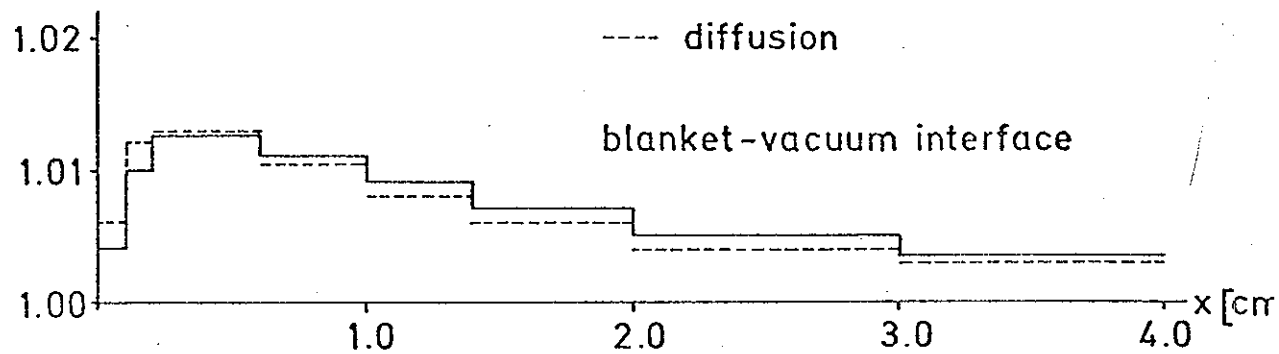
$R(\text{corr.})/R(\text{uncorr.})$



$R(\text{corr.})/R(\text{uncorr.})$



$R(\text{corr.})/R(\text{uncorr.})$



Reaction rate ratios for capture in U-238

References

- /1/ E. Teuchert, R. Breitbart, Jülich, Jül-551-RG
- /2/ L.W. Nordheim, G.F. Kuncir, GA-2527 (1961)
- /3/ H. Jonas, M. Kloth, R. Hecker, Jülich; Proc. Reaktortagung Karlsruhe (1973)
- /4/ P.H.Kier, A.A. Robba, Report ANL-7326 (1967)
- /5/ F.R. Askew et al., J. Brit. Nucl. Energy Soc. 5, 564 (1966)
- /6/ G. Arnecke et al., Report KFK-2190 (1975) documented by V. Brandl
- /7/ H. Küsters, KFK-1632 (1973)
- /8/ P.E. McGrath, E.A. Fischer, KFK-1557 (1972)
- /9/ D. Wintzer, Proc. of IAEA Conf. on Reactor Physics, Karlsruhe, 1967
- /10/ F. Helm et al. KFK-1399 (1971)
- /11/ H. Huschke, KFK-1353 (1971)
- /12/ R. Schröder et al., KFK-847 (1968)
- /13/ H.A. Böhme, private Communication (1976)