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EUROPEAN ATOMIC ENERGY COMMUNITY — EURATOM

RECENT INVESTIGATIONS CONCERNING THE INFLUENCE OF NON-UNIFORM TEMPERATURE DISTRIBUTION IN DOPPLER EFFECT CALCULATIONS

by

G. BLÄSSER and W. MATTHES

1963

Joint Nuclear Research Center
Ispra Establisment - Italy
Reactor Physics Department
Applied Mathematical Physics Service

PAPER PRESENTED AT THE « VIII CONGRESSO NUCLEARE »
ROME (ITALY) 17-23.6.1963

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RECENT INVESTIGATIONS CONCERNING THE INFLUENCE OF NON-UNIFORM TEMPERATURE DISTRIBUTION IN DOPPLER EFFECT CALCULATIONS

SUMMARY

To study the influence of nonuniformities in the temperature distribution inside the fuel rods the Doppler coefficient has been calculated by direct integration of the narrow-resonance formulas for a single resonance for a slab lattice. Also, a Monte Carlo method has been developed which allows the calculation of the total temperature coefficient of non-uniformly heated fuel in the region of unresolved resonances; in this method the details of the resonance structure are determined by sampling from the statistical level and widths-distributions. Preliminary results of both theories will be presented.

1 — INTRODUCTION

The practical importance of the exact knowledge of the change in resonance absorption due to the Doppler-broadening of the resonance lines is well known. For this reason the Doppler-effect has been considered in almost all computations of effective resonance integrals [1]. Extensive tabulations of the functions that appear in calculations of this type have been given by Dresner [2] for the calculation of homogeneous resonance integrals and by Adler and Nordheim [3] for the heterogeneous case. However, in all these treatments of Doppler-broadening the assumption was made that the thermal motion of the absorbing nuclei can be described by a single value of the parameter "fuel temperature".

In modern power reactor projects, especially in the case of intermediate and fast assemblies, the trend to high power densities and the use of rather poor thermal conductors as for instance uranium oxide as fuel make it necessary to provide for the non-uniform temperature distribution in the fuel.

The first part of this paper deals with the calculation of the absorption in a single resonance line at energy E_r in the case of a plane lattice, where plates containing the resonance absorber alternate with plates of some coolant or moderator.

2 — EXPRESSIONS FOR THE CROSS SECTIONS

The cross section Σ_1 in the coolant plates is assumed constant in space and lethargy and corresponding to pure scattering only. Inside the plates we have a mixture of some pure scattering materials, with constant cross section Σ_m, and the resonance absorber, with atomic density N and a total microscopic cross section σ_t, which is the sum of a potential scattering cross section σ_p (constant), and of the energy dependent cross sections σ_a (absorption), σ_{sr} (resonance scattering) and σ_i (interference term between resonance and potential scattering). However, the interference term is usually rather small and we shall therefore neglect it. The shape of the resonant parts of the cross sections for a Doppler broadening corresponding to a temperature T is given by

$$\sigma_a(E,T)=\sigma_r\frac{\Gamma_\gamma}{\Gamma}\psi(\theta,x) \qquad \sigma_{sr}=\sigma_r\frac{\Gamma_n}{\Gamma}\psi(\theta,x) \tag{1}$$

where

$$\psi(\theta,x)=\frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{\exp\left[-\frac{\theta^2}{4}(x-y)^2\right]}{1+y^2}dy \tag{2}$$

$$\theta=\frac{\Gamma}{\Delta} \qquad \Delta=\left(\frac{4\,E_r\,kT}{A+1}\right)^{1/2} \tag{3}$$

$$\sigma_r=4\,\pi\,\lambda\!\!\!^{-2}\,g_J\frac{\Gamma_n}{\Gamma} \qquad x=\frac{E-E_r}{\Gamma/2} \tag{4}$$

and where the other symbols have their usual meaning (k = Boltzmann's constant, A = mass number of the resonance absorber, Γ_n, Γ_γ, Γ = neutron, radiation and total width, respectively, g_J = statistical weight factor for the compound state of total angular momentum J, $2\,\pi\lambda\!\!\!^{-}$ = wave lenght associated with the relative motion neutron-nucleus).

In the case we are considering the temperature is not uniform across the absorber plates, but is a function of the coordinate z normal to the plates.

By solving the equation of heat conduction for a uniform heat source density Q, a surface temperature T_1, a mean coefficient of heat conduction κ and a plate thickness a, we obtain

$$T=T_1+\frac{z(a-z)}{2\,\kappa}Q \tag{5}$$

Inserting this expression in eq. (3), Δ,θ and therefore $\psi(\theta,x)$ become functions of z. Henceforth we write $\sigma(E,z)$ instead of $\sigma(E,T(z))$.

3 — EXPRESSION FOR THE RESONANCE INTEGRAL

We treat the resonance absorption in the narrow resonance approximation, which is valid if the practical width of the resonance (i.e. the width of the energy interval, in which the resonant part of the cross section exceeds the potential part) is narrow with respect to the mean loss of energy per collision with any of the nuclei present in the reactor. For uranium this condition is valid in the kev-range.

We have two contributions to the absorption: the first comes from the neutrons which had their last collision in the absorber plates; the second consists of the neutrons slowed down in the coolant. We start with the first part. Since the resonance has been assumed to be narrow we have a spatially and lethargically uniform source density $\Sigma_p\phi$ in the absorber plates, where

$$\Sigma_p = N\sigma_p + \Sigma_w \tag{6}$$

and ϕ is the flux per unit of lethargy above the resonance (c.f. the discussion in Chapter V of [1]). Let $K\,(z,z,E)dz'$ be the probability that a neutron generated with energy E in a plate at a point z makes its next collision in an interval dz' at a point z' in one of the plates (in each plate the coordinate z measures the distance from the left-hand surface). Now the total absorption rate of the neutrons of energy E generated in one plate becomes

$$\Sigma_p\phi \int_0^a\int_0^a K(z,z',E)h(z',E)dz\,dz' \tag{7}$$

where

$$h(z,E) = \frac{N\sigma_a(z,E)}{\Sigma_a(z,E)} = \frac{\Gamma_\gamma}{\Gamma}\,\frac{\Sigma_0(z,E)-\Sigma_p}{\Sigma_0(z,E)} \tag{8}$$

and

$$\Sigma_0(z,E) = N\sigma_t + \Sigma_m = N\sigma_r\psi\left(\theta(z),\frac{E-E_r}{\Gamma/2}\right) + \Sigma_p \tag{9}$$

Let us now consider the neutrons which originate in the moderator. Let $P(z,E)dz$ be the probability that a neutron of energy E generated in the region between two of the plates makes its next collision at a point z in the interval dz in one of the plates.

The source strength in this region is $\Sigma_1\phi$.

Therefore the contribution of these neutrons to the total absorption is

$$(b\Sigma_1)\phi\int_0^a P(z,E)h(z,E)dz \tag{10}$$

b being the thickness of the coolant layer between two fuel plates. By definition [1], the effective resonance integral I of the line is then given by

$$NI = \int_0^\infty \frac{dE}{E}\left\{a\Sigma_p\int_0^1\int_0^1 K(\rho,\rho',E)h\,(\rho',E)d\rho\,d\rho' + b\Sigma_1\int_0^1 h(\rho,E)P(\rho,E)d\rho\right\} \tag{11}$$

with $\rho = z/a$.

As the result of the straight-forward calculations one obtains

$$NI=\int_0^\infty \frac{dE}{E}\int_0^1 \frac{d\omega}{\omega}\frac{\Gamma_\gamma}{\Gamma}\left\{\Sigma_p\left[\omega\left(1-R(\omega,E)\frac{1-\exp(-\Sigma_1 b/\omega)}{1-\exp(-T(E)/\omega)}\right)\right.\right.$$

$$\left.-\Sigma_p a\left(R_1(\omega,E)+R^2(\omega,E)\frac{\exp(-\Sigma_1 b/\omega)}{1-\exp(-T(E)/\omega)}\right)\right] \qquad (12)$$

$$\left.+\frac{1-\exp(-\Sigma_1 b/\omega)}{1-\exp(-T(E)/\omega)}\left[\frac{\omega^2}{a}(1-\exp(-s(a,E)/\omega)-\Sigma_p\omega R(\omega,E)\right]\right\}$$

where

$$\omega=\cos\vartheta$$

ϑ being the angle between the direction of flight of the neutron and the positive z-axis,

$$s(z,E)=\int_0^z \Sigma_0(z',E)dz'$$

$$T(E)=s(a,E)+b\Sigma_1$$

$$R(\omega,E)=\frac{1}{a}\int_0^a \exp(-s(z,E)/\omega)dz$$

$$R_1(\omega,E)=\frac{1}{a^2}\int_0^a dz.\exp(-s(z,E)/\omega)\int_0^z dz'\exp(s(z',E)/\omega)$$

These formulae have been programmed for the IBM 7090 (this work was done in collaboration with SOMEA, Milano).

As an example, we calculated the resonance integrals for the following cases: (isolated plate, $\Sigma_1 b \gg 1$)
$a=0.3$ cm, $b=10$ cm, $\Sigma_1=1.5$ cm^{-1}, $E=1000$ eV, $\Gamma_n=0.07$ eV, $\Gamma_\gamma=0.03$ eV, $\sigma_r=1950$ barn, $N=0.0223\times10^{24}$ nuclei/cm^3, $\Sigma_p=0.65$ cm^{-1}. If one plots the values of the effective resonance integrals NI (cm^{-1}) for different central and surface temperatures as functions of the mean temperature

$$\bar{T}=T_1+\frac{2}{3}(T_{\max}-T_1)$$

one obtains a smooth curve (see Fig. 1). This indicates that for the given resonance the mean temperature can be used as "effective temperature" for the calculation of the Doppler effect.

In similar calculations for the Doppler effect in a non-moderating fuel plate (Infinite Absorber-Mass Approximation) Keane [4] has found some differences between mean and effective temperature. It seems that in the present case the considerable slowing-down in the fuel produces a more uniform absorption in the different regions of the fuel element. Further calculations are planned to resolve these questions.

4 — MONTE CARLO PROGRAM
FOR THE CALCULATION OF THE DOPPLER-COEFFICIENT IN A FAST REACTOR

In principle we only have to calculate the multiplication-factor K for a given temperature-distribution. For this we start a number of fission-neutrons N_0 in the reactor and count how many fission neutrons (N_1) are produced in the next generation, ($K=N_0/N_1$).

To trace a fission neutron through its life from collision point to collision point we have to answer two questions:

a) what happens at a collision point and

b) where is the next collision point ?

5 — ENERGY-DEPENDENCE OF CROSS SECTIONS

To find out what happens at a collision point, we need the probabilities for the different kind of reactions possible, i.e. the cross sections. As we take the shape of the reactions cross section to be given by the Breit-Wigner resonance formula, we can calculate their values if we know all the parameters which characterize a resonance (position and reaction width). These parameters are not known for the energy range that contributes most to the Doppler coefficient in fast reactors; we have only some information about the statistical behaviour of these parameters, that is, we know only their distribution functions. (Chisquare distributions for resonance spacing and for reactionwidth's. The necessary parameters for these distributions were taken from [5].) By a random sampling we simply have to pick out of these distribution functions a set of parameters for the resonance in question and calculate the cross sections numerically out of the analytical formulas.

6 — SPACE-DEPENDENCE OF CROSS SECTIONS

We come now to the other question: where is the next collision point ? This is a purely geometrical problem and depends on the geometrical configuration. For our example we took a reactor consisting of fuel needles (about 3 mm diameter) arranged in a square lattice (lattice pitch about 4 mm).

We pick now out of the distribution e^{-d} a value d for the optical distance up to the next collision point and find the geometrical distance s out of the relation:

$$d = \int_0^s \Sigma(w_0 + nt)dt \qquad \begin{array}{ll} w_0: & \text{last collision point} \\ n\ : & \text{direction after collision} \end{array} \tag{13}$$

if the cross section is space dependent. This is in fact the case for our example as the temperature in the fuel needles shows a parabolic behaviour and the cross sections depend from the temperature. This dependence is such, that we have with increasing temperature a decrease of the cross section in the center of the resonance and an increase of the cross section in the wings of the resonance. If we now move from the surface of the rod towards the center we have an increase of the temperature and therefore an increase or decrease of the cross section. This leads us to the assumption that we can approximate the real spatial dependence of the cross section also by a parabolic shape:

$$\Sigma(r) = a_0 r^2 + b_0 \tag{14}$$

If we insert this quadratic dependence of the cross section from the distance from the center of the rod in equation (1), we find the following relation of third degree between the number of mean free path and the geometrical distance (for a flight in a fuel element):

$$d = as^3 + bs^2 + cs \tag{15}$$

where the parameters a, b and c depend from the last collision point w_0 and the direction n in which the neutron escapes.

Now we have the necessary tools available to build up a neutron history and to calculate the multiplication factor K for a given temperature-distribution. Then we have to change the temperature-distribution somewhat and to calculate K again to find another value K' which can lie within the range of the statistical error of K. We may not therefore simply perform the difference $K' - K$ to find the effect of the temperature-change on the multiplication factor. But it is possible to calculate the difference ΔK directly with the Monte Carlo method.

7 — DIFFERENTIAL EFFECTS

We calculate the number F of fission neutrons produced by one starting neutron, then we change the temperature and let the neutron again run on the same geometrical path producing hereby another number F' of new fission neutrons. The difference $F' - F$ gives us a direct contribution to ΔK. The calculation of F' can be done for the same geometrical path in the changed temperature case by properly modifying the weight of the neutron during its flight:

The probability that the neutron makes its next collision in ds after traversing the distance s is given by $e^{-d_0(s)}\Sigma_0\, ds$, ($d_0(s)$ is the number of mean free path's up to the next collision point, Σ_0 is the total cross section at the next collision point). If we change the temperature this probability is given by $e^{-d_1(s)}\Sigma_1\, ds$. As we take for both cases the same geometrical path, that means we sample in the "changed" case out of the distribution function for the unchanged case, we have to provide the neutron with a weight

g in such a way that: $e^{-d_0(s)}\Sigma_0 ds.g = e^{-d_1(s)}\Sigma_1 ds$. It is this factor g with which we have to multiply the weight of the neutron running for the changed case when entering a collision process and then we proceed in the usual way.

8 — RESULTS

With this method we have made some calculations for the following situations:

Diameter of the fuel elements:	0.317 cm				
Distance of the fuel elements:	0.368 cm (square lattice)				
Composition of the fuel elements:	10% U235, 90% U238				
Temperatures:	T_{center} (°c)	700	1000	1300	1500
	$T_{surface}$ (°c)	500	500	500	500

In our special example the neutrons started with an energy of about 10 Kev and were followed until they passed 1 Kev, (we made the assumption that we have no contribution to the Doppler effect in the energy range above 10 Kev). The results are shown in fig. 2. These results can be used to give an answer to the problem of the mean temperature. If we want to replace $K=K(T_c,T_s)$ *by* $K=K(T_m)$ where the mean temperature T_m should be calculated out of the temperatures T_s and T_c by a procedure that is independent of T_s and T_c we are led to the condition: $\Delta K/\Delta T_c = \text{const.}\ \Delta K/\Delta T_s$.

As this proportionality is not shown in Fig. 2, we conclude that it is not possible to introduce a mean temperature in the way above. For the type of reactor considered, one has to employ two Doppler-coefficients $\Delta K/\Delta T_s$ and $\Delta K/\Delta T_c$ and we showed that it is possible to calculate these quantities with the Monte Carlo method.

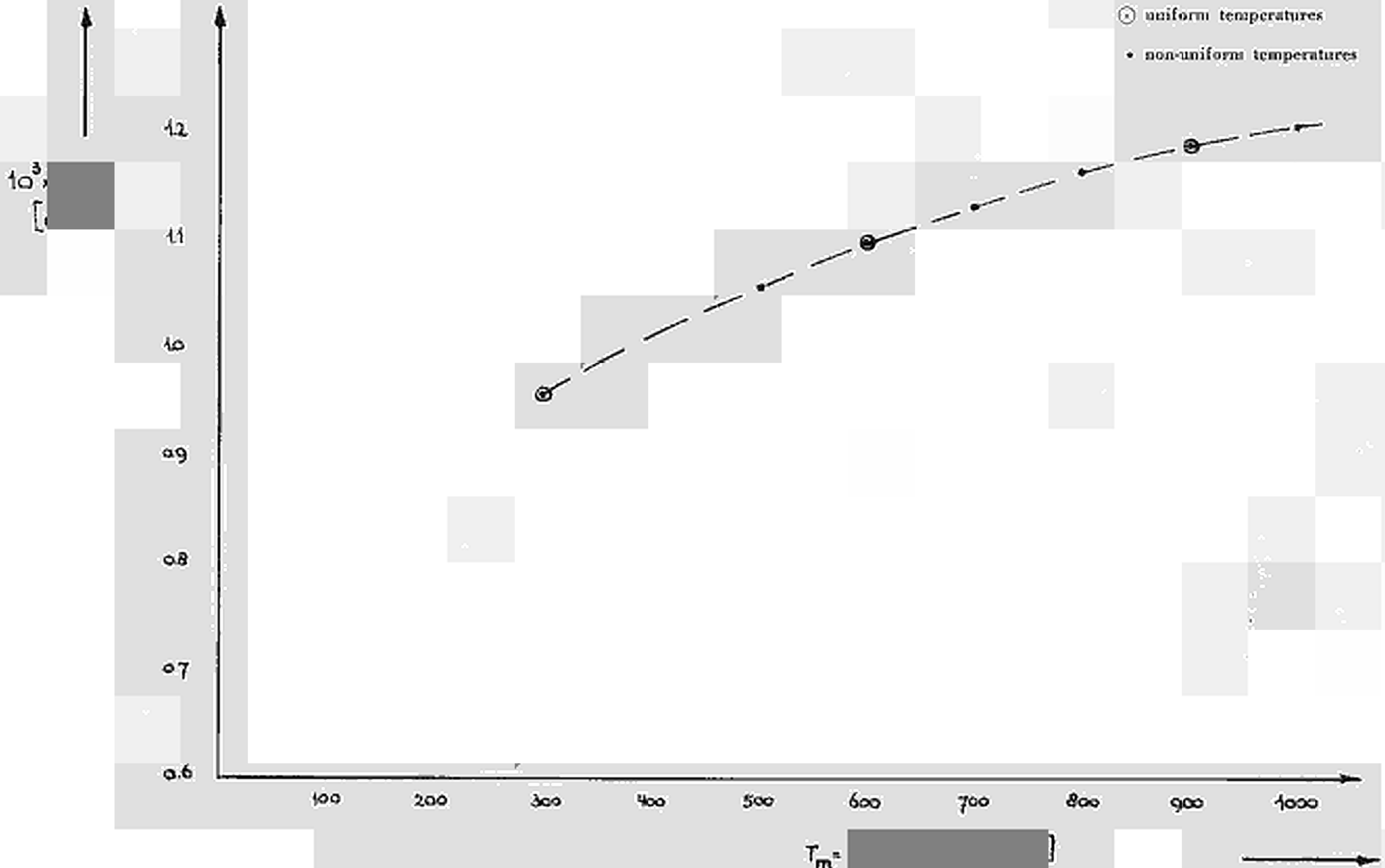

Fig. 1: Resonance integral of a single line as function [redacted]

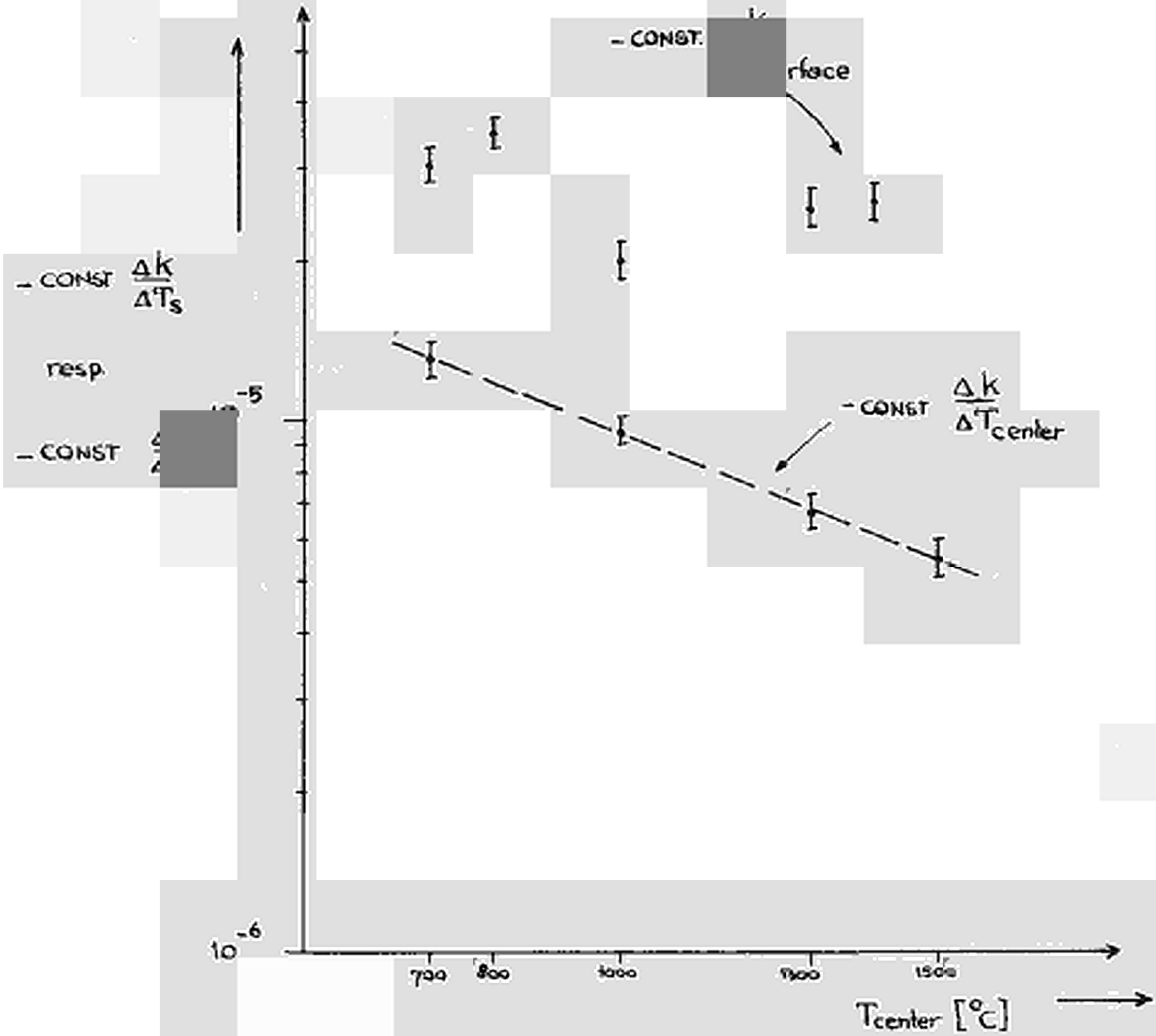

Fig. 2: Values for const. $\frac{\Delta K}{\Delta T}$ as a function of the central temperature ($T_{surface}=500°C$).

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