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CALCULATION OF D_2O MODERATED LATTICES BY BASIC METHODS

by

B. STURM

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For the calculation of D$_2$O moderated, organic cooled natural uranium lattices a calculational procedure is proposed on the basic of most refined reactor codes available at Ispra. For the calculation of fast group constants the GAM-I multigroup program is used. Weighting factors to take into account the heterogenity of the lattice, cell are calculated by the DSN program for macro- and micro-

cell. For the calculation of thermal cross sections the THERMOS-code is used and the disadvantage factors for the different materials in the cell are obtained by a one group calculation using the DSN program.

On the basis of this procedure an analysis of critical experiments done by AECL for a 7 UO$_2$ rod organic cooled fuel element, is performed.

Reasonable agreement is found for material buckling as well as for measured thermal disadvantage factors, initial conversion ratio and fast fission ratio.

EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

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Contents

1. Introduction

Sinoe the seoond Geneva oonferenoe the following "olassioal" approaoh
to the physioal oaloulation of D_2O moderated lattioes has turned out
to be the most promising one.

On the basis of a very simple model of the neutron oyole, the two
group-four faotor formula, a set of formula and oross seotions
is established that provides the oaloulation of f, ε , p, L^2 and L_s^2 .
Together with experimental values of the material Buokling B^2 whioh
is measured in exponential or critical assemblies for a range of
different lattioe oonfigurations, an adjusted value of the thermal
reproduotion faotor η is obtained from the relation

$$\eta' = \frac{(1+ B^2 L_s^2)(1+ B^2 L^2)}{\varepsilon f p}$$

This speoial approaoh was used by the swedish group of the AB
Atomenergi in Sweden [1] . Other groups for example the Saolay
group in Franoe adjusted both η and the resonanoe integral of
U^{238}[2] where-as the Savannah river group in USA adjusts the reso-
nanoe integral only [3] .

The reaotor oodes written on the basis of this philosophy have the
great advantage of small computer time and are therefore very suitable
for optimisation studies. The aoouraoy of suoh oaloulations is ra-
ther good and allows reaotivity prediotions with an uncertainty of
the order of $\Delta \varrho = \pm 0.005$ for the oold olean reaotor.

An evident disadvantage of this simplified approaoh is the faot
that it is limited to the range of lattioe oonfigurations for whioh
the B^2-oorrelation has been performed.

Furthermore the extrapolation to the hot irradiated reaotor re-
mains a rather problematic business.

As concernes the Orgel-project the situation is the following:

The simplified reactor-physics-code CAROLINA I [4] developped at Ispra which is based on the French correlation method [2] with some additional features arising from the presence of organic in the fuel element has been compared with results of critical-Euratom experiments for nine different lattice configurations with UO_2 fuel and Monoisopropyl-diphenyl coolant. A fairly satisfactory agreement has been found for this comparison and also for organic cooled 7 rod UO_2 elements that where measured in the ZED-2 reactor in Chalk River [5].

Although these promising results justified first optimisation of the ORGEL-reactor on the basis of the CAROLINA I-code, it seemed worthwhile to look for an independent and more sophisticated calculation method, especially to calculate the reactivity balance and the temperature coefficients of the ORGEL-reactor in the hot irradiated condition.

For this reason we have investigated the possibility of applying the most refined codes already available at Ispra for lattice calculation of organic-heavy water reactors.

Due to the fact that the used computer codes start from basic cross section-data and do not contain any adjustment to integral experiments, we will call this approach in contrast to the above mentioned "correlated" methods, "basic" methods.

2. The method

The simplified methods make no attempt to calculate the actual space- and energy dependent neutron-flux $\emptyset$ (E,$\vec{r}$) in the unit cell of the lattice. A consequence of this is the necessity to adjust certain parameters of the calculation.

A basic approach has therefore to start with a more refined calculation of the space- and energy- dependence of neutron-flux and -current. Once this dependence is known, cell averaged group constants can be calculated and the macroscopic behaviour of the neutron-flux can be treated by a few-group approach.

To derive the connection between material buckling and group constants (in view of doing comparison with experiments), we start from the two group equations assuming that the group constants are averaged over the actual neutron spectrum in the unit cell. The joining point between the two energy groups is more or less arbitrary but for unirradiated lattices it should lie below the lowest U^{238} resonance and so high that upscattering of neutrons from thermal group into fast group is very small.

We have then

$$D_1 \Delta \phi_1 - (\Sigma_{a_1} + \Sigma_{1\to 2}) \phi_1 + (\nu\Sigma_f)_1 \phi_1 + (\nu\Sigma_f)_2 \phi_2 = 0$$
$$D_2 \Delta \phi_2 - \Sigma_{a_2} \phi_2 + \Sigma_{1\to 2}\phi_1 = 0 \tag{1}$$

where D, Σ_a, $\Sigma_{1\to 2}$ and $\nu\Sigma_f$ denote space- and energy-averaged values over the flux spectra in the two energy groups.

The solutions of this set of inhomogeneous differential equations for a bare reactor are of the type

$$\Delta \phi_i + B^2 \phi_i = 0 \quad , \quad i = 1,2 \tag{2}$$

where B^2 is the geometrical buckling.

Introducing (2) into (1) we obtain the critical equation

$$(D_1 B^2 + \Sigma_{a_1} + \Sigma_{1\to 2} - (\nu\Sigma_f)_1)(D_2 B^2 + \Sigma_{a_2}) = (\nu\Sigma_f)_2 \cdot \Sigma_{1\to 2} \tag{3}$$

With the abbreviations

$$\Sigma_{a_1} + \Sigma_{1\to 2} = \Sigma_R$$

$$L_1'^2 = \frac{D_1}{\Sigma_R - (\nu\Sigma_f)_1} \qquad ; \qquad L_1^2 = \frac{D_1}{\Sigma_R} \tag{4}$$

$$L_2^2 = \frac{D_2}{\Sigma_{a2}}$$

$$K_\infty = \frac{(\nu\Sigma_f)_2}{\Sigma_{a2}} \frac{\Sigma_{1\to2}}{\Sigma_R} + \frac{(\nu\Sigma_f)_1}{\Sigma_R}$$

we obtain from (3)

$$B^2 = -\frac{1}{2}\left(\frac{1}{L_2^2} + \frac{1}{L_1'^2}\right) + \sqrt{\frac{1}{4}\left(\frac{1}{L_2^2} + \frac{1}{L_1'^2}\right)^2 + \frac{K_\infty - 1}{L_2^2 L_1^2}} \tag{5}$$

It can be easily shown, that K_∞ is the usual infinite multiplication factor defined as

$$K_\infty = \frac{\text{number of neutrons produced in the cell}}{\text{number of neutrons absorbed in the cell}} \tag{6}$$

If we write K_∞ in (4) in the form

$$K_\infty = \frac{\iint_0^{E^*} \nu\Sigma_f(E,\nu)\,\phi(E,\nu)\,dE\,d\nu}{\iint_0^{E^*} \Sigma_a(E,\nu)\,\phi(E,\nu)\,dE\,d\nu} \cdot \frac{\iint_{E^*}^{\infty} \Sigma_{1\to2}(E,\nu)\phi(E,\nu)\,dE\,d\nu}{\iint_{E^*}^{\infty}[\Sigma_a(E,\nu)+\Sigma_{1\to2}(E,\nu)]\phi(E,\nu)\,dE\,d\nu} +$$

$$+ \frac{\iint_{E^*}^{\infty} \nu\Sigma_f(E,\nu)\,\phi(E,\nu)\,dE\,d\nu}{\iint_{E^*}^{\infty}[\Sigma_a(E,\nu)+\Sigma_{1\to2}(E,\nu)]\phi(E,\nu)\,dE\,d\nu} \tag{7}$$

with E^* denoting the energy limit between fast and thermal group and notice, that for neutron balance reasons

$$\iint_0^{E^*} \Sigma_s(E,v)\, \phi(E,v)\, dE\, dv = \iint_{E^*}^{\infty} \Sigma_{1\to 2}(E,v)\, \phi(E,v)\, dE\, dv \tag{8}$$

we obtain

$$\iint_{E^*}^{\infty} [\Sigma_a(E,v)+\Sigma_{1\to 2}(E,v)]\, \phi(E,v)\, dE\, dv = \iint_{E^*}^{\infty} \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv +$$

$$+ \iint_0^{E^*} \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv = \iint_0^{\infty} \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv$$

and from (7)

$$K_\infty = \frac{\iint_0^{\infty} v\, \Sigma_f(E,v)\, \phi(E,v)\, dE\, dv}{\iint_0^{\infty} \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv} \qquad \text{in agreement}$$

with definition (6).

To check the validity of our method we can compute from equation (5) the material buckling and compare with experimental values. But even if the agreement between experimental and calculated B^2-values has been found to be sufficient, this may be due to a fortuitous cancellation of systematic errors in the different group constants. To check also this "internal consistency" of our method, we have choosen for our comparison some experiments of the AECL group in which for a 7 rod UO_2 organic cooled bundle, apart from the material buckling B^2, also the thermal disadvantage factors, the initial conversion ratio δ_0 and the fast fission ratio R where measured [6] .

To do this comparison we have to derive the relation between γ_o, R and the group constants.

γ_o is defined as

$$\gamma_o = \frac{\text{fast and thermal captures in } U^{238}}{\text{fast and thermal absorptions in } U^{235}} \qquad (9)$$

Let us define:

$$c_2^{28} = \int_o^{E^*}\!\!\int \Sigma_c^{28}(E,v)\, \phi(E,v)\, dE\, dv \qquad (10a)$$

$$c_1^{28} = \int_{E^*}^{\infty}\!\!\int \Sigma_c^{28}(E,v)\, \phi(E,v)\, dE\, dv \qquad (10b)$$

$$A_2^{25} = \int_o^{E^*}\!\!\int \Sigma_a^{25}(E,v)\, \phi(E,v)\, dE\, dv \qquad (10c)$$

$$A_1^{25} = \int_{E^*}^{\infty}\!\!\int \Sigma_a^{25}(E,v)\, \phi(E,v)\, dE\, dv \qquad (10d)$$

then we have

$$\gamma_o = \frac{c_1^{28} + c_2^{28}}{A_1^{25} + A_2^{25}} \qquad (11)$$

Considering the relations:

$$\frac{(v\Sigma_f)_2}{\Sigma_{a2}} = \frac{\int_o^{E^*}\!\!\int v\,\Sigma_f(E,v)\, \phi(E,v)\, dE\, dv}{\int_o^{E^*}\!\!\int \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv} = \eta \cdot f \qquad (12)$$

$$\eta_2^{25} = \frac{\int_o^{E^*}\!\!\int v\,\Sigma_f^{25}(E,v)\, \phi(E,v)\, dE\, dv}{\int_o^{E^*}\!\!\int \Sigma_a^{25}(E,v)\, \phi(E,v)\, dE\, dv} = \frac{\overline{\sigma_f}^{25}}{\overline{\sigma_a}^{25}}\, v_2^{25} \qquad (13)$$

$$\int_{E^*}^{\infty}\!\!\int \Sigma_{1\to2}(E,v)\, \phi(E,v) = Q_2 = (1 + B^2 L_2^2)\int_o^{E^*}\!\!\int \Sigma_a(E,v)\, \phi(E,v)\, dE\, dv \qquad (14)$$

we obtain from (12) (13) and (14)

$$A_2^{25} = \frac{\frac{(\nu \Sigma_f)_2}{\Sigma_{a2}} Q_2}{\eta_2^{25} (1 + B^2 L_2^2)} \tag{15}$$

defining

$$p = \frac{Q_2}{Q_2 + A_1^{28} + A_1^{25} + C_1^{str}} = \frac{\Sigma_{1 \to 2}}{\Sigma_R} \tag{16}$$

and

$$s = \frac{\nu F_1^{25} + \nu F_1^{28}}{Q_2 + A_1^{28} + A_1^{25} + C_1^{str}} = \frac{(\nu \Sigma_f)_1}{\Sigma_R} \tag{17}$$

where

$$C_1^{str} = \int_{E^*}^{\infty} \int \Sigma_c^{str}(E, \nu) \phi(E, \nu) \, dE \, d\nu \qquad \text{are the fast captures}$$

in structure material of the cell and νF_1^{25} and νF_1^{28} are the fast fissions of U^{25} and U^{28}

$$\nu F_1^{25} = \int_{E^*}^{\infty} \int \nu \Sigma_f^{25}(E, \nu) \phi(E, \nu) \, dE \, d\nu$$

$$\nu F_1^{28} = \int_{E^*}^{\infty} \int \nu \Sigma_f^{28}(E, \nu) \phi(E, \nu) \, dE \, d\nu$$

we have from (16) and (17)

$$Q_2 = \frac{p \left[\nu F_1^{25} + \nu F_1^{28} \right]}{s} \tag{18}$$

Inserting (18) into (15) we obtain

$$A_2^{25} = \frac{\eta f p \left[\nu F_1^{25} + \nu F_1^{28} \right]}{\eta_2^{25} \cdot s (1 + B^2 L_2^2)} \tag{19}$$

From (19) and from the relation

$$\frac{C_2^{28}}{A_2^{25}} = \frac{N^{28}}{N^{25}} \cdot \left(\frac{\overline{\sigma_c}^{28}}{\overline{\sigma_a}^{25}}\right)_2$$

(20)

where $\overline{\sigma}^i$ is the cross section of nucleus i averaged over the thermal spectrum and N^i is the number density, we obtain from (11) using the critical equation (3).

$$\gamma_\circ = \frac{\dfrac{N^{28}}{N^{25}}\left(\dfrac{\overline{\sigma_c}^{28}}{\overline{\sigma_a}^{25}}\right)_2 + \dfrac{C_1^{28}}{\nu F_1^{25}+\nu F_1^{28}} \cdot \dfrac{\eta_1^{25} \cdot \jmath}{1-\jmath+B^2 L_1^2}}{1 + \dfrac{A_1^{25}}{\nu F_1^{25}+\nu F_1^{28}} \cdot \dfrac{\eta_2^{25} \cdot \jmath}{1-\jmath+B^2 L_1^2}}$$

(21)

Let us now define

$$p^{28} = \frac{Q_2}{Q_2+C_1^{28}} = \frac{\Sigma_{1\to 2}}{\Sigma_{1\to 2} + \dfrac{\iint_{E^*} \Sigma_c^{28}(E,v)\phi(E,v)\,dE\,dv}{\iint_{E^*}\phi(E,v)\,dE\,dv}}$$

(22)

$$p^{25} = \frac{Q_2}{Q_2+A_1^{25}} = \frac{\Sigma_{1\to 2}}{\Sigma_{1\to 2} + \dfrac{\iint_{E^*} \Sigma_a^{25}(E,v)\phi(E,v)\,dE\,dv}{\iint_{E^*}\phi(E,v)\,\phi(E,v)\,dE\,dv}}$$

(23)

so we can write

$$\frac{C_1^{28}}{\nu F_1^{25}+F_1^{28}} = \frac{C_1^{28}}{Q_2+A_1^{28}+A_1^{25}+C_1^{str}} = \frac{C_1^{28}+Q_2-Q_2}{Q_2+A_1^{28}+A_1^{25}+C_1^{str}}$$

$$= \frac{(C_1^{28}+Q_2)(1-p^{28})}{Q_2+A_1^{28}+A_1^{25}+C_1^{str}} = \frac{1-p^{28}}{p^{28}} \cdot \frac{Q_2}{Q_2+A_1^{25}+A_1^{28}+C_1^{str}} = \frac{1-p^{28}}{p^{28}}\,p$$

(24)

and similarly we obtain

$$\frac{A_1^{25}}{F_1^{25} + F_1^{28}} = \frac{1-p^{25}}{p^{25}} \cdot p \tag{25}$$

Inserting (24) and (25) into (21) we obtain finaly

$$f_o = \frac{\dfrac{N^{28}}{N^{25}} \left(\dfrac{\overline{\sigma}_c^{28}}{\overline{\sigma}_a^{25}} \right)_2 + \dfrac{\eta_2^{25}}{1-\vartheta + B^2 L_1^2} \cdot p \cdot \dfrac{1-p^{28}}{p^{28}}}{1 + \dfrac{\eta_2^{25}}{1-\vartheta + B^2 L_1^2} \cdot p \cdot \dfrac{1-p^{25}}{p^{25}}} \tag{26}$$

All quantities in equation (26) can be simply calculated from the group constants as we will show later on the discussion of the calculation of the group constants.

Let us now derive a similar equation for the fast fission ratio R:

R is defined as

$$R = \frac{\text{number of fissions in } U^{238}}{\text{number of fissions in } U^{235}} \tag{27}$$

or

$$R = \frac{F_1^{28}}{F_1^{25} + F_2^{28}} \tag{28}$$

with $\qquad F_j^i = \iint \Sigma_f^i (E, \vec{r}) \, \phi(E, \vec{r}) \, dE \, d\upsilon \qquad$ taking the energy

integration over energy group j.

With

$$F_2^{25} = \frac{\eta_2^{25}}{\nu_2^{25}} \cdot A_2^{25} \tag{29}$$

and A_2^{25} from equation (19) using the relation

$$\frac{\eta\,fp}{1+L_2^2B^2} = 1-s + B^2L_1^2 \qquad \text{we obtain}$$

$$F_2^{25} = \frac{1-s+B^2L_1^2}{\nu_2^{25}}\,\frac{\nu F_1^{25} + \nu F_1^{28}}{s} \tag{30}$$

Inserting this into (28) we have for R

$$R = \frac{F_1^{28}}{\dfrac{1-s+B^2L_1^2}{\nu_2^{25}}\cdot\dfrac{\nu F_1^{25} + \nu F_1^{28}}{s}+ F_1^{25}} \tag{31}$$

When the fast spectrum is calculated F_1^{28}, F_1^{25}, F_1^{25} and F_1^{28} can be obtained easily.

2.1. Calculation of the fast group constants

The General Atomics Multigroup program GAM-I [7] was used for the calculation of the fast neutron spectrum. GAM-I treats the slowing problem in the consistent P_1-approximation. The P_1 equations of the energy dependent Boltzmann equation are integrated over quarter lethargy units from 10 MeV to 0.414 MeV yielding a total of 68 groups. The code provides group constants for maximum of 32 broad groups. Furthermore for each case a set of one-fast-group constants is provided. For each broad-group a different leakage factor can be provided. A further advantage over other existing multigroup programs is the possibility of treating heterogeneous lattices by providing for each nucleus in each broad-group so called "self shielding" factors i.e. weighting factors of the flux in each group to take into account the heterogeneity effects.

Resonance absorption is treated by the Nordheim method [8]. Resonance parameters are included in the library tape and resonance integrals are calculated for each of the 68 groups.

For our calculations the fast energy range has been devided
from 10 MeV to $E^* = 0.683$ eV into 11 broad-groups with the
following energy limits:

Tab. 1

Group No.	lower energy	lethargy interval
1	3.68 MeV	1.0
2	1.35 MeV	1.0
3	0.388MeV	1.25
4	0.111MeV	1.25
5	31.8 KeV	1.25
6	9.12 KeV	1.25
7	0.961KeV	2.25
8	130 eV	2.0
9	17.6 eV	2.0
10	5.04 eV	1.25
11	0.683 eV	2.0

The treatment of the heterogeneity of the cell proceeds as follows:

Let us devide the cell into N subregions (fuelpins, canning, coolant,
tubes and moderator) and let us define the mean flux in region n by

$$\phi_n(E) = \frac{1}{V_n} \int \phi(E, \nu) \, d\nu \qquad n = 1 \ldots N \qquad (32)$$

Then we can write the integral for a nucleus k

$$I_k = \int_{E^*}^{10 \text{ MeV}} \int_{\text{Cell}} \Sigma_k(E, \nu) \, \phi(E, \nu) \, dE \, d\nu \qquad (33)$$

as

$$I_k = \sum_{n=1}^{N} \sum_{l=1}^{L} N_{kn} \cdot \sigma_{kl} \cdot V_n \cdot \phi_{nl} \cdot \Delta u_l \qquad (34)$$

where we have devided the energy range $E^* = 0.683$ eV to 10 MeV into L subgroups l, with

$$\int_{group\ \ell} \bar{\phi}_n (E)\, \sigma_k (E)\, dE = \bar{\phi}_{nl}\, \sigma_{k\ell}\, \Delta u_\ell \qquad (35)$$

Let $\bar{\phi}_l$ be the mean cell flux in energy group l and $\sum\limits_{n=1}^{N} N_{kn} \cdot V_n \Big/ V_{cell} = N_k$

the numberdensity of nucleus k in the cell.

Then we can write

$$I_k = \sum_{n=1}^{N} \sum_{\ell=1}^{L} N_{kn} \sigma_{k\ell} V_n \frac{\bar{\phi}_{n\ell}}{\bar{\phi}_\ell} \cdot \bar{\phi}_\ell\, \Delta u_\ell \cdot \frac{\sum\limits_{n=1}^{N} N_{kn} V_n}{\sum\limits_{n=1}^{N} N_{kn} V_n} \qquad (36)$$

or with

$$w_{k\ell} = \frac{\sum\limits_{n=1}^{N} N_{kn} V_n \cdot \frac{\bar{\phi}_{n\ell}}{\bar{\phi}_\ell}}{\sum\limits_{n=1}^{N} N_{kn} V_n} \qquad (37)$$

$$I_k = \int_{E^*}^{10 MeV} \int \Sigma_k (E,\vec{r})\, \phi(E,\vec{r})\, dE\, dv = \sum_{\ell=1}^{L} \sigma_{k\ell}\, w_{k\ell}\, \bar{\phi}_\ell\, \Delta u_\ell \cdot N_k\, V_{cell} \qquad (38)$$

We see, that by introducing the weighting factors $w_{k\ell}$ for each group l and each nucleus k we can reduce the heterogeneous problem to a homogeneous one for the calculation of the energy dependent mean cell flux $\bar{\phi}_\ell$.

The mean-flux ratios $\overline{\Phi_{n\ell}}/\Phi_{\ell}$ which are needed for the calculation of the weighting factors $W_{\kappa\ell}$ are calculated separately by a 11-group cell calculation for micro- and macro-cell. The macro-cell is formed by the fuel rod bundle homogenised inside of the rubberband surface, a layer containing outer coolant and tube (s) and the moderator region. The micro-cell is composed of a single fuel pin and associated canning and coolant. The code used for this cell-calculation was the DSN-code of Carlson and Bell [9] . The cross sections needed where calculated from a homogeneized GAM-I calculation. A subroutine written by M. Quiqmelle of Euratom made it possible to punch the output of GAM-I 11 group cross sections on cards which directly could be introduced in DSN.

So the calculation of fast group constants turns out to be a iteration process which is illustrated in Fig. 1.

From a homogeneous GAM-I calculation ($W_{\kappa\ell} = 1$ for all k and l) we obtain a set of microscopic 11-group cross sections $\overline{\sigma}_{\kappa\ell}$ for the nuclei. From two DSN-calculations for micro- and macro-cell we obtain the weighting factors $W_{\kappa\ell}$ that now are introduced into GAM-I obtaining a new set of $\overline{\sigma}_{\kappa\ell}$ et. cet. As final result we obtain from GAM-I a set of 1-group fast constants Σ_{a1} , $\Sigma_{1\rightarrow 2}$, $(\nu\Sigma_f)_1$, D_1 and for each nucleus a set of 11-group microscopic cross sections that are multiplied by the weighting factors $W_{\kappa\ell}$. Moreover we obtain for 11 broad groups the values $\alpha_\ell = \phi_\ell \cdot \Delta u_\ell$ and so we can calculate the reaction integrals I_k that are necessary for the calculation of γ_0' and R:
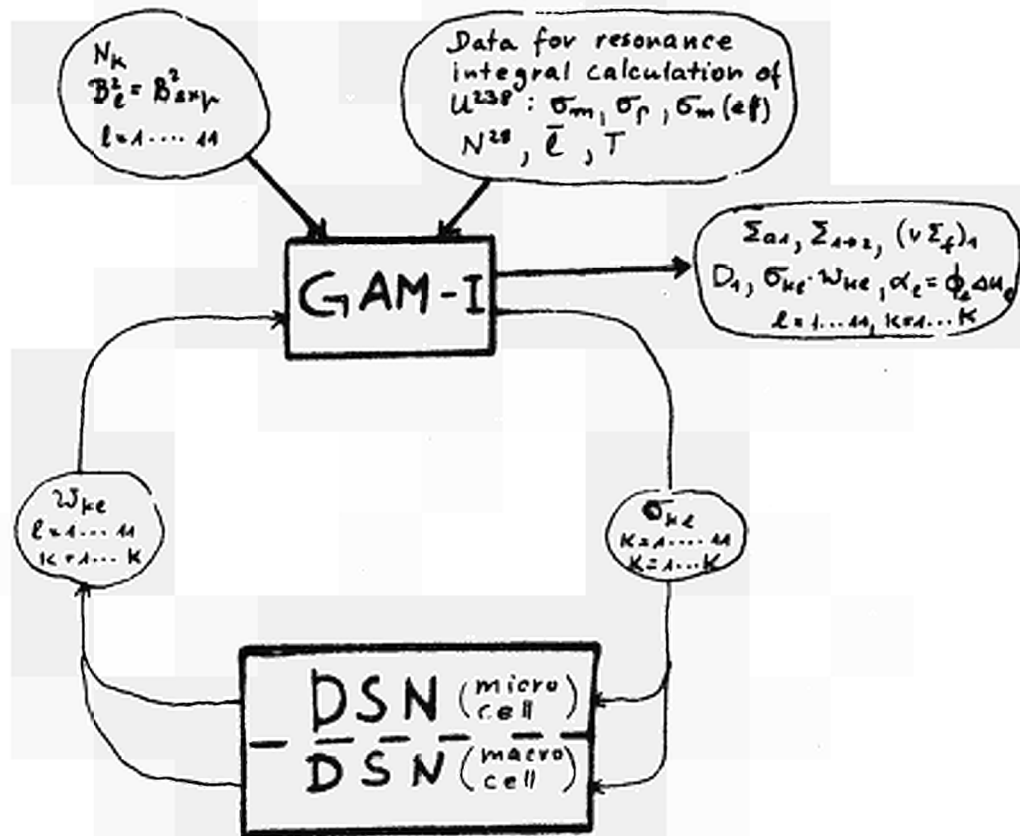
Fig. 1: Iteration process for the calculation of fast group constants

N_k numberdensity of nucleus k in cell, k = 1 ... K

B_1^2 Buckling in broad group l, l = 1...11

         (for bare reactor $B_1^2 = B^2$ for all l, for comparison with experiments B^2 was set equal to B_{exp}^2)

σ_m moderator cross section per resonance absorber atom

σ_r total scattering cross section per resonance absorber atom

$\sigma_m(ef)$ effective cross section for unresolved resonance integral calculation

N^{28} lumped nuclear absorber density

$\bar{l}$ mean chord length in the absorber lump

T   absolute temperature of absorber

$$C_1^{28} = N_{28} \ V_{cell} \cdot \sum_{\ell=1}^{44} \sigma_{c\ell}^{28} \ w_{\pi\iota\ell} \ \bar{\phi}_{c\ell} \ \Delta u_\ell \tag{39a}$$

$$A_1^{25} = N_{25} \ V_{cell} \cdot \sum_{\ell=1}^{44} \sigma_{a\ell}^{25} \ w_{\imath\varsigma\ell} \ \bar{\phi}_{c\ell} \cdot \Delta u_\ell \tag{39b}$$

$$F_1^{28} = N_{28} \ V_{cell} \cdot \sum_{\ell=1}^{44} \sigma_{f\ell}^{28} \ w_{\imath\iota\ell} \ \bar{\phi}_{c\ell} \cdot \Delta u_\ell \tag{39c}$$

$$vF_1^{28} = N_{28} \ V_{cell} \cdot \sum_{\ell=1}^{44} v\sigma_{f\ell}^{28} \ w_{\imath\iota\ell} \ \bar{\phi}_{c\ell} \cdot \Delta u_\ell \tag{39d}$$

$$vF_1^{25} = N_{25} \ V_{cell} \cdot \sum_{\ell=1}^{44} v\sigma_{f\ell}^{25} \ w_{\imath\varsigma\ell} \ \bar{\phi}_{c\ell} \cdot \Delta u_\ell \tag{39e}$$

In our calculations we stopped the iteration process GAM-I-DSN after the second GAM-I run, calculating the weighting factors W_{kl} only once. This was justified by the fact, that the microscopic cross sections σ_{kl} from the homogeneous GAM-I case showed practically no difference compared with the σ_{kl} of the heterogeneous GAM-I case indicating that the mean cell energy dependent flux was quite insensetive to the weighting factors W_{kl}. On the contrary: the macros-copic one-fast group constants of the heterogeneous GAM-I calculation were very different from the homogeneous calculation especially in the case of the fast absorption Σ_{al} and the fast fission $(v\Sigma_f)_A$ indicating the importance of heterogeneous treatment of a lattice fast spectrum in the case of D_2O moderated natural uranium lattices.

2.2. Resonance absorption

In order to calculate the fast absorber cross section of nuclei with strong resonances (U^{238}, Th^{232}) GAM-I uses the narrow resonance (NR) approach for resonances with practical width smaller than the mean energy loss by collision with an absorber nucleus.

For wide resonances the narrow-resonance infinite absorbermass (NRIA) approximation is applied. The following constants have to be provided for input:

σ_m the moderator cross section per absorber atom (σ_m = 0 for pure metal, $\sigma_m = 2\sigma_p^0 x$ for UO_2) and $^m THO_2$

σ_p total potential scattering cross section per absorber atom

$\bar{l}$ = $\dfrac{4\ V_{abs}}{S_{eff}}$ = mean cord length in the absorber lumps. V_{abs} being the total volume and S_{eff} the effective surface of the absorber.

In the case of bundle elements composed of several fuel rods, l has been calculated using the well known formula of Carlvik and Pershagen 9 :

$$S_{eff} = S_{rb} + \gamma \cdot S_i \qquad (40)$$

with $\qquad \gamma = 2\sum_M \rho_i (1 - P_c (\Sigma_M \cdot \rho_i))$

S_{rb} being the rubberband surface of the bundle

S_i the inner surface

Σ_M the potential macroscopic scattering cross section of the medium between the rods of the bundle

ρ_i radius of the gratest circle which could be inscribed between neighbouring fuel rods

P_c collision probability for a cylinder of radius and cross section

For the unresolved region the NR-approximation is employed throughout. The statistical distribution of neutron width is taken into account and the equivalence theorem is used to eliminate the surface integration by substituting $\sigma_p + \dfrac{4}{\bar{l}N}$ for σ_p in the volume absorption term for the resonance integral, N being the lumped nuclear density of absorber atoms.

The contribution of resonances above 30 KeV and p-states below
30 KeV is not included in the GAM-I code, as has been shown by
comparison with experimental data of Hellstrand [9] for U-metall
and UO_2 and calculated values for UC reported by Vernon [10]. For
this reason the U^{238} capture cross section for input in the DSN-
calculation have been corrected by adding 0.8 barns for energies
above 30 KeV and about 0.9 barns (depending from $\frac{S}{M}$ - values for the
bundle) below 30 KeV. A corresponding correction of the macroscopic
1-fast group cross section of U^{238} was applied to the results of
the heterogeneous GAM-I calculation.

2.3. Calculation of thermal group constants

For the calculation of space- and energy dependent thermal flux
and neutron density and to obtain average thermal cross sections
we used the THERMOS-program written by Honeck [11] , [12] .
THERMOS solves the space- and energy dependent Boltzmann equation
numerically by dividing the energy-resp. space interval into
maximal 30 resp. 20 intervals. The assumption of isotropic neutron
scattering and neutrondensity is used in the code and the transport-
approximation is made for all nuclei except Hydrogen. For the cal-
culation of the scattering matrices the free gas model has been
used in the formulation of Brown-St. John for Deuterium and Hydro-
gen. It has been pointed out by Honeok and Kaplan [13] that diffi-
culties appear in the interpretation of fine structure measurements
with THERMOS in cases when hydrogeneous material is present in the
cell. It was assumed, that the reason for this are the assumptions
of isotropic scattering and isotropic neutron density and the use
of the free gas model for the hydrogen scattering. In order to
avoid this difficulties which may also appear in the case of or-
ganic materials in the cell we have choosen the following proce-
dure to calculate the thermal fine-structure:

1. For a given cell configuration a THERMOS-calculation is per-
   formed and microscopic cross sections for each material aver-
   aged over the energy range $0-E^*$ are obtained.
   Brown-St. John-type scattering kernels are used for all materials
   assuming that in the case of D_2O moderated cells the free gas
   model used for the hydrogen in the organic is sufficient for
   the calculation of the energy dependence of the neutron
   density.

2. Using this cross sections a $DSN-S_6$ one group calculation is made
   to obtain flux disadvantage factors and from this cell averaged
   macroscopic cross sections are calculated. In the case of
   bundle elements a microscopic DSN-calculation is performed
   to obtain the microflux correction.

In the THERMOS-calculation the scattering cross section of hydrogen
is used, whereas in the DSN calculation the transport approximation
is made for hydrogen scattering.
To check this procedure we have performed calculations of relative
thermal neutron densities in a lattice for which experiments have
been made by Boeuf and Tassan [14] .

The fuel element consisted of a 44 mm diameter U metal rod sheated
by 1.0 mm Al with 45 mm inner diameter. Between Al-sheath and
a pressure tube of 1.5 mm thickness there was a 5 mm thick layer
of Monoisopropyl-diphenyl $C_{15} H_{16}$. The neutron density distribution
was measured by Dy^{164} - activation and the epithermal correction
using point - by - point values of the Cd-ratio was applied to ob-
tain the thermal neutron density below the cut-off at 0.1265 eV.

Tab. 2 shows the results:

Table 2: **Comparison of measured and calculated relative thermal neutron densities**

Method	Uranium	Al-sheath	Organic	Al-tube	Moderator
THERMOS $\sigma^H = 22.7+39.0 \cdot v_0^{035}$ Meff = 2.1	1.000	1.509	2.227	2.795	3.718
DSN using THERMOS cross sections with transport approximation for hydrogen	1.000	1.4920	2.0874	2.5937	3.6499
Experiment	1.00	1.450	2.099 ± 0.01	2.693	-

The results in the first line of the table were obtained by using simply the output neutron densities of the THERMOS calculation. The values of the second line were calculated with the above mentioned procedure: the cross sections of the THERMOS calculation were used for all materials except for hydrogen, for which the transport cross section was taken. With these cross sections a one group DSN calculation was performed. The output-fluxes were multiplied by the corresponding values of the mean neutron celocities obtained by THERMOS and the relative numberdensities were calculated for each material. The transport cross section for hydrogen was obtained by applying the Radkowski presoription to the energy dependent scattering cross section used in the THERMOS-code.

From the comparison of the different results with the experimental values it is obvious that the neglection of the anisotropic scattering of hydrogen leads to errors in the flux disadvantage factors and therefore in the thermal utilisation which are of the order of several per mille.

The calculation of the thermal group constants $(\nu \Sigma_f)_2$, Σ_{a2}, D_2 proceeds now in a straight forward manner: the mean fluxes $\bar{\phi}_i$ in each material i of the cell and the corresponding volumes V_i and cross section Σ_i are used to calculate the group constants from:

$$(\nu \Sigma_f)_2 = \frac{\nu_2^{25} \Sigma_f^{25} V_f \bar{\phi}_f}{\sum_i V_i \phi_i}$$

$$\Sigma_{a2} = \frac{\sum_i \Sigma_{ai} V_i \bar{\phi}_i}{\sum_i V_i \phi_i}$$

$$D_2 = \frac{1}{3\Sigma_{tr}} \quad \text{with} \quad \Sigma_{tr} = \frac{\sum_i \Sigma_{tri} V_i \phi_i}{\sum_i V_i \phi_i}$$

where $\nu_2^{25} = 2.43$ is the number of fast neutrons produoed per thermal fission in U^{235}. The thermal utilisation f oan be obtained from

$$f = \frac{(\nu \Sigma_f)_2}{\Sigma_{a2}} \cdot \frac{1}{\eta}$$

with

$$\eta = \frac{\nu_2^{25} \Sigma_{f2}^{25}}{\Sigma_{a2}^{25}}$$

and the thermal diffusion length is given by

$$L_2^2 = \frac{D_2}{\Sigma_{a2}}$$

3. Comparison with experiments

In order to check the calculation methods described in section 2 we have calculated the physical quantities δ_θ, R, $(\phi_i/\phi_u)_{th}$ and B^2 for a organic-cooled 7 rod UO_2 fuel element for which measurements of these quantities have been performed in Canada ([6]) in the ZED-2 reactor, for three lattice pitches. The detailed description of the fuel element are reported in the paper of G.A. Beer and D.W. Hone [15] . The UO_2 was in the form of cylindrical pellets with 2.40 cm diameter and average density of 10.2 g/cm^3. The pellets were stacked in a Al-tube with inside diameter of 2.44 cm, a wall thickness of 0.051 cm and a length of 46.5 cm to form a cluster rod. Seven such rods were bundled together in a hexagonal pattern with a center to center spacing of 2.667 cm. Five bundles loaded into a Al pressure tube with a inside diameter of 8.256 cm and a wall thickness of 0.089 cm formed one fuel assembly. The gap between the UO_2 in adjacent clusters was 1.63 cm. Additional aluminium due to tie rods, rod and plugs and endplates had to been taken into account in the calculations. This was done homogenizing all materials over the total bundle length which was 47.31 cm.

The material filling the coolant channel was an organic liquid (HB-40) with the bruttoformula $C_{18}H_{22.04}$ and density 1.01 g/cm^3 at 20° C. The measurement of B^2, $\gamma_\bullet$, R and the disadvantage factors were performed in a hexagonal pattern at three pitches: 19,22 and 28 cm.

3.1. Initial conversion ratio

The experimental method for the determination of the initial conversion ratio is described by Tunniciffe et. al. in [16] . It is based on the determination of relative fission rates and relative N_p^{239} production by foil activation techniques. By intercomparison of the activities from thin sections of fuel simultaneously irradiated in a fuel element and in a pure thermal

flux and correcting for fission product activity of U^{238} one obtains the ratio of Np^{239} production over U^{235} fission in the rod to the N^{239} production over U^{235} fission in a purely thermal spectrum:

$$\wp = \frac{(N^{239}prod)_{rod}}{(U^{235}fin.)_{rod}} : \frac{(N_p^{239} prod)_{th}}{(U^{235} fin.)_{th}}$$

multiplying $\wp$ by $\left(\frac{\Sigma_a^{?8}}{\Sigma_a^{?5}}\right)_{th}$ and by $\frac{(1+\alpha)_{th}}{(1+\alpha)_{rod}}$ which can be obtained from Westcott's report C RRP-960 Tunnicliffe et. al. obtain the initial conversion ratio

$$\gamma_o = \wp \cdot \left(\frac{\Sigma_a^{?8}}{\Sigma_a^{?5}}\right)_{th} \cdot \frac{(1+\alpha)_{th}}{(1+\alpha)_{rod}}$$

which gives after cancellation

$$\gamma_o = \frac{(N^{239} prod) \; rod}{\Sigma_a^{25} \; rod} = \frac{\text{number of } N_p^{239} \text{ atoms produced}}{\text{number of } U^{235} \text{ atoms destroid}}$$

The relative error of γ_o obtained by this method is estimated to be $\pm$ 0.5%.

Table 3 gives the comparison of calculated and experimental results.

Table 3: Comparison of calculated and experimental values of the initial conversion ratio

Pitch (cm)	γ_o (element average)	γ_o (mid bundle value)	γ_o (experimental mid bundle value)
19	0.809	0.819	0.824 $\pm$ 0.004
22	0.769	0.778	0.784 $\pm$ 0.004
28	0.729	0.735	0.737 $\pm$ 0.004

The χ_o -values of the first column are calculated using the axialy homogenized nuclear densities to take into account the bundle end effects. The experiments however were performed in the middle of the bundle, therefore the values given in the second column have been corrected to the midbundle density of U^{238}, to have a better comparison with the experimental situation. It should be pointed out that the error limits of the calculated values coming from the uncertainty of nuclear constants entering into formula (26) are of the order of magnitude of $\pm$ 4%. Keeping this in mind the agreement between calculation and experiment appears to be surprisingly good.

3.2. Fast fission ratio

The experimental technique for the measurement of fast fission ratios has been discribed by Hanna and Tunnicliffe [17]. The measured quantity is the ratio

$$\delta'(t) = \frac{\text{fission product } \gamma\text{-activity from depleted U-foil}}{\text{fission product } \gamma\text{-activity from natural U-foil}}$$

$$= \frac{A_D^{25}(t) + A_D^{28}(t)}{A_N^{25}(t) + A_N^{28}(t)} \tag{47}$$

Let N_D^i resp. N_N^i (i = 28,25) be the numberdensity of nucleus i in the depleted resp. natural uranium foil then we have

$$A_D^{25}(t) = \alpha(t)\, N_D^{25} \int \sigma_f^{25} \phi\, dE$$

$$A_D^{28}(t) = \beta(t)\cdot N_D^{18} \int \sigma_f^{25} \phi\, dE$$

$$A_N^{25}(t) = \alpha(t)\cdot N_N^{25} \int \sigma_f \phi\, dE \tag{48}$$

$$A_N^{28}(t) = \beta(t)\, N_N^{18} \int \sigma_f \phi\, dE$$

Introducing this and

$$\delta = \frac{N_N^{18} \int \sigma_f^{28} \phi\, dE}{N_N^{25} \int \sigma_f^{25} \phi\, dE} \tag{49}$$

one obtains for δ the expression

$$\delta = \frac{\alpha(t)}{\beta(t)} \cdot \frac{\dfrac{N_N^{28} \cdot N_D^{25}}{N_D^{28} \cdot N_N^{25}} - \gamma(t)\dfrac{N_N^{28}}{N_D^{28}}}{\dfrac{N_N^{28}}{N_D^{28}}\gamma(t) - 1} \tag{50}$$

An auxiliary experiment is necessary to determine the ratio $P(t) = \alpha(t)/\beta(t)$. This is done by measuring in a double chambered fission counter the ratio of fissions occuring in a natural foil to fissions in depleted foil and counting also the fission product activity apearing in this irradiation.

In table 4 the experimental results obtained from this method are compared with theoretical values which were computed from equation (31).

Table 4: Comparison of calculated and experimental values of the
fission ratio

Pitch (cm)	R (element average)	R (experimental)
19	0.0572	0.059 ± 0.002
22	0.0552	0.054 ± 0.002
28	0.0536	0.0531± 0.0015

Again the agreement between calculation and experiment is very satisfactory: the calculated values lie within the experimental errorlimits. The variation of the fast fission ratio with the pitch, which is due to fast interaction between fuel rod bundles and to spectral effects, is less pronounced as in the experiment. This may be due to the fact that we have taken the fission source distribution flat over the fuel rod bundle in calculating the weighting factors by DSN. Nevertheless, the error due to this effect will be smaller than ± 2 mk.

3.3. Thermal disadvatage factors

Neutron activation distributions were determined for the 7 rod bundle placed in a central lattice site. The detectors used were Mn-Ni foils placed between fuel pellets and Mu-Ni wires located in the fuel pellets and at various positions in the coolant region and moderator. The total activities so obtained were corrected for macroscopic flux variation and Mn-resonance activation to obtain the total neutron density distribution throughout the cell. The average neutron densities in the various cell material were then found by graphical integration. The measurements were done at a moderator temperature of about 25° C; the errors are $\pm$ 2%.

Table 5

Material	pitch 19		pitch 22		pitch 28	
	$\left(\frac{n_i}{n_{UO_2}}\right)^{therm}_{calc}$	$\left(\frac{n_i}{n_{UO_2}}\right)^{tot.}_{exper}$	$\left(\frac{n_i}{n_{UO_2}}\right)^{therm}_{calc.}$	$\left(\frac{n_i}{n_{UO_2}}\right)^{tot.}_{exper}$	$\left(\frac{n_i}{n_{UO_2}}\right)^{therm.}_{calc.}$	$\left(\frac{n_i}{n_{UO_2}}\right)^{tot.}_{exper.}$
UO_2	1.000	1.00	1.000	1.00	1.000	1.00
Al-sheath	1.106	1.088	1.106	1.104	1.108	1.120
Organic	1.392	1.400	1.403	1.422	1.415	1.416
tie rods	1.513	1.554	1.511	1.545	1.481	1.596
Al-tube	1.845	1.750	1.874	1.819	1.903	1.900
Moderator	2.304	2.170	2.448	2.310	2.657	2.585

In table 5 the experimental results are compared with calculation which were performed using the procedure outlined in section 2.3. Before doing a comparison it must be mentioned that the calculated quantities for several reasons have not the same physical meaning:

1. the calculated quantities are relative thermal neutron densities, whereas the experiment determines total densities.

2. the experiments were performed in the middle of the bundle whereas the calculations were performed for an axialy homogenized element.

3. the calculated values belong to a moderator temperature of 20° C whereas the experiments were performed at 25°C.

Estimations using experimental determined values of the spectral parameter r and of flux peaking factors for the different materials which are also reported in $\begin{bmatrix} 6 \end{bmatrix}$, show, that the effects of point 1. and 2. cancel out each other approximately and that the correction due to effect 3. is of the order of 1 % in the case of the moderator disadvantage factor.

So the direct comparison seems to be justified at least within the experimental errors which are of the order of ± 2%. One sees, that the calculations agree with the experiments for Al-sheath and for organic whereas for Al-tube and moderator there is a overestimation of the neutrondensities especially at small pitches which is of the order of maximal 5%.

3.4. Material Buckling

Experimental material backlings for the 7 UO_2 rod bundle with organic coolant obtained by Beer and Hone $\begin{bmatrix} 5 \end{bmatrix}$ by the flux-mapping technique are compared in table 6 with values which were calculated from equation (5).

Table 6: Comparison of material buckling

Pitch (cm)	B^2_{exp} (m^{-2})	B^2_{calc} (m^{-2})
19	3.24 ± 0.1	3.455
20	3.44 ± 0.1	-
22	3.48 ± 0.1	3.477
24	3.26 ± 0.1	-
28	2.68 ± 0.1	2.632

In Fig. 2 the B^2 values are plotted as function of the pitch. To have a comparison with results obtained by a correlation method, B^2 calculated by the CAROLINA-I code are given by curve 2. It is seen that both calculational methods tend to overestimate the material buckling at small pitches. In the case of the "basic" method (curve 1) the reason for this is not known, but one could suppose that it may be due to some incorrectness in treating hydrogen because the relative hydrogen content is greatest at small pitch. To clarify this more comparisons have to be done for organic cooled lattices.

4. Conclusions

An attempt has been made, to calculate physical data of heavy water moderated organic colled lattices simply by using refined reactor physics codes available at Ispra. First calculations utilizing the codes GAM-I, DSN and THERMOS were performed for a lattice of $7UO_2$-rod organic cooled fuel elements at three pitches and gave promising results. The calculated fast fission ratios agreed with the experiments within the error limits. In the case of initial conversion ratio the maximal deviation of the calculation was 0.75%. The calculated material bucklings agree sufficently well with experiments except at the smallest pitch where the maximal deviation is of the order of 6.6% corresponding to an error in reactivity of the order of ~ 4.1 ‰.
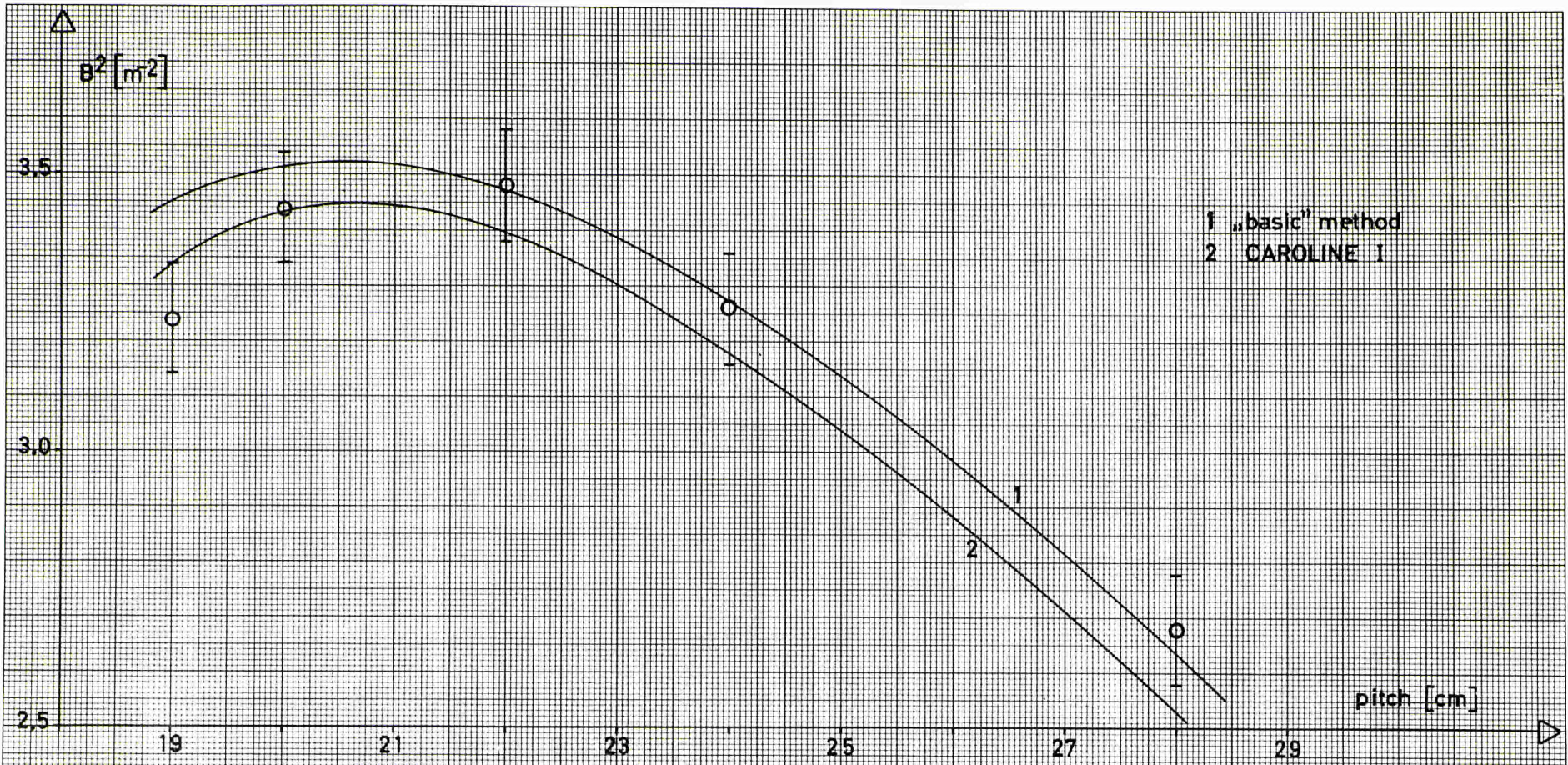
Fig. 2 :   COMPARISON OF CALCULATED AND EXPERIMENTAL BUCKLINGS

7 UO_2- rod organic cooled element

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