INDC (HUN) - 4/G

KFKI-70-14 RPT

426

Z. Szatmáry

J. Valkó

GRACE - A MULTIGROUP FAST NEUTRON SPECTRUM CODE

Hungarian Academy of Sciences

CENTRAL
RESEARCH
INSTITUTE FOR
PHYSICS

BUDAPEST

GRACE - A MULTIGROUP FAST NEUTRON SPECTRUM CODE

Z. Szatmáry and J. Valkó

1. Introduction

GRACE is a multigroup fast neutron spectrum code. In writing it, the main emphasis has not been laid on originality but rather on using a formalism which is thoroughly tested and which proved to work satisfactorily in generating few-group constants for diffusion calculations. Hence the basic algorithm of GRACE is a slight modification of that of the BIGG-II code [3] which in turn is an advanced version of the BIGG-I and BPG codes [1, 2] having MUFT as the common ancestor.

Code GRACE solves the asymptotic neutron transport equation in slab geometry using the Greuling-Goertzel approximation for the slowing down neutron source. The code permits the use of both B_1 and P_1 approximations. In the multigroup structure of GRACE a thermal group has been included making an iteration to criticality of the slab possible.

Group constants as well as energy limits for the thermal energy group must be specified in input. For the treatment of resonance absorption and fission two options are available:

- The same formalism has been built in GRACE which is used in BIGG-II, based on empiric resonance integrals and Dancoff factors. In case of uranium metal and UO_2 the formulae of Hellstrand have been included in the code.

- Lattice resonance integrals for all of the resonance materials present in the slab investigated can be given in input separately for all of the groups containing resonances. In this way resonance groups can be treated like any other fast group.

Another important feature of GRACE is a great simplicity of input preparation which has become possible by the inclusion of a subroutine /called DATAPREP/ doing all the lattice homogenization, calculation of resonance integrals, Dancoff-factors, fast advantage factors, etc. based on formulae of ref. [4].

Besides fuel regions, non-fuel regions such as reflectors can be treated by GRACE as well. For reflector regions, the source term is the leakage from the region previously treated and space dependence of the neutron spectrum is described by an artificial energy dependent buckling as introduced in ref. [3] .

The code GRACE is member of a reactor physics model. Its main results are group constants for few-group diffusion calculations, for one hand, and it uses results of other codes, for the other hand: thermal constants from THERMOS [7] and lattice resonance integrals from RIFFRAFF [6] when using the second resonance option mentioned above.

This report describes the mathematical model on which the code GRACE is based in Section II., it provides a user's manual in Section III. As to the physical fundamentals, only the very digit is given here and the reader is referred to refs. [1-5]. In order to facilitate to look up things in these references, the notations established in them will be retained here.

II. The physical model of GRACE

GRACE is an essentially zero-dimensional code. By solving the asymptotic reactor equation, it calculates the neutron flux and current in a bare homogeneous slab. Finiteness of the slab is taken into account by introducing a buckling. As pointed out by Radkowsky [5] , this treatment results in good few group constants in the core independently of whether it is reflected or not, although, near the boundary of regions of different material compoitions, the spectrum is space dependent. To explain this, it can be argued that, this space dependence affects only a small part of the core while the spectrum is space dependent far inside the reflector. For this reason, in contrast to the core, the reflector can not be characterized by a single neutron spectrum. A correct treatment of systems consisting of several different regions would be a one-dimensional finite difference algorithm which would give the neutron spectrum in several points of the system. But there is an alternative possibility suggested by ref. [3] to introduce <u>some</u> space dependence also into a zero-dimensional treatment. If the buckling is allowed to depend on neutron energy, the attractive formalism of the asymptotic reactor theory can be preserved and, at the same time, the resulting equations still contain some aspects of space dependence. Of course, such a treatment is a synthetic one and its adequacy can be justified only by comparison with experiment.

Now for real systems, GRACE is used in the following way. The regions of different material composition are treated one by one. The core is taken first. Core regions have their own neutron source /i.e. fission/ so that they can be considered independently from the others. Reflector regions have their neutron field supplied from the neighbouring regions. Thus in reflectors, the source term is related to the leakege from the core or from the preceding reflector region.

All these points will be cleared up in detail in the following sections.

II.1. The fundamental equations

Write the transport equation for slab geometry in the following form [1]:

$$\mu \frac{\partial \phi(\mu,u,x)}{x} + \Sigma^T(u)\ \phi(\mu,u,x) = \int_0^{2\pi} d\Theta \int_{-1}^{1} d\mu_o\ \Sigma^o(\mu_o,u')\cdot\phi(\mu',u',x) +$$

$$+ \frac{1}{k_{eff}} \frac{f(u)}{2} \int_0^{\infty} du' \int_{-1}^{1} d\mu'\ \nu(u')\ \Sigma^F(u')\ \phi(\mu',u',x) +$$

$$+ \frac{1}{2} \int_0^{\infty} du' \int_{-1}^{1} d\mu'\ \Sigma^I(u',u)\ \phi(\mu',u',x) \qquad /1/$$

where

- x is the spatial coordinate,
- u is the lethargy,
- Θ is the azimuthal angle,
- μ is the cosine of the angle of neutron direction and x axis,
- $\phi(\mu,u,x)$ is tha angular flux at space point x of neutrons of lethargy u and of direction cosine μ ,
- $\Sigma^T(u)$ is the total cross section,
- $\Sigma^o(\mu_o,u')$ is the transfer cross section for elastic scattering which changes the direction of a neutron of lethargy u' by an angle whose cosine is μ_o . This angle corresponds to a lethargy change of $(u-u')$,

$f(u)$ is the fission spectrum normalized to 1,

$\Sigma^F(u)$ is the fission cross section,

$\nu(u)$ is the mean number of neutrons produced in fissions, caused by neutrons of lethargy u,

$\Sigma^I(u',u)$ is the transfer cross section for inelastic scattering which changes the neutron lethargy from u' to u,

k_{eff} is the static eigenvalue or the effective multiplication constant.

If a trial function of the form

$$\phi(\mu,u,x) = e^{-iBx}\ \psi(\mu,u) \qquad /2/$$

is inserted in Eq. /1/ and $\psi(\mu,u)$ is expanded in a series of Legendre polinomials as

$$\psi(\mu,u) = \sum_{m=o}^{\infty} \frac{2m+1}{4\pi}\ \psi_m(u)\ P_m(\mu)\ , \qquad /3/$$

then a straightforward calculation shows /see Ref. [1]/ that Eq. /1/ can be rewritten in the following way:

$$\Sigma^T(u)\ \psi_o(u) = L_o(u) + iB\ \psi_1(u) + S(u) + I(u)\ , \qquad /4a/$$

$$\Sigma^T(u)\ h(u)\ \psi_1(u) = L_1(u) + \frac{iB}{3}\ \psi_o(u)\ . \qquad /4b/$$

In Eqs. /4/

$$\psi_o(u) = 2\pi \int_{-1}^{1} \psi(\mu,u)\ d\mu \qquad /5a/$$

is the neutron spectrum and

$$\psi_1(u) = 2\pi \int_{-1}^{1} \mu\psi(\mu,u)\ d\mu = iJ(u) \qquad /5b/$$

where J u is the neutron current. Furthermore,

$$L_m(u) = 2\pi \int_{-1}^{1} \psi_m(u')\ P_m(\mu_o)\ \Sigma^o(\mu_o,u')\ d\mu_o \qquad /6/$$

is the slowing down source by elastic scattering i.e. $L_o(u)$ is the number of neutrons which reach lethargies between u and u+du in unit of time by elastic scattering collision. The physical significance of $L_1(u)$ is much harder to tell; it is connected with the anisotropy of the slowing down process in the laboratory system. The slowing down source by inelastic scattering collisions is given by

$$I(u) = \int_0^\infty \Sigma^I(u',\mu)\ \psi_o(u')\ du' \quad , \qquad /7/$$

i.e. I(u) has the same physical significance for inelastic scattering as $L_o(u)$ for elastic scattering. S(u) is the source of neutrons produced by fission. Because Eq. /1/ together with all the succeeding equations is homogeneous, the neutron flux may be normalized in such a way that

$$\int_0^\infty \nu(u)\ \Sigma^F(u)\ \psi_o(u)\ du = k_{eff} \ . \qquad /8/$$

Consequently, in Eq. /4a/ one has

$$S(u) = f(u) \ . \qquad /9/$$

Finally,

$$h(u) \equiv 1 \qquad /10a/$$

in P_1 approximation while in B_1 approximation

$$h(u) = \frac{1}{3}\left(\frac{B}{\Sigma^T(u)}\right)^2 \frac{\beta}{1-\beta} \qquad /10b/$$

where

$$\beta = \begin{cases} \dfrac{\Sigma^T(u)}{B}\ \text{arctg}\ \dfrac{B}{\Sigma^T(u)} & \text{for real } B \qquad /10c/ \\[2ex] \dfrac{\Sigma^T(u)}{B}\ \log\left|\dfrac{1+B/\Sigma^T(u)}{1-B/\Sigma^T(u)}\right| & \text{for imaginary } B \qquad /10d/ \end{cases}$$

In case of reflectors, Eqs. /4/ and /10/ have a slightly modified form which will be given in Section II.5.

If one considers that $iB\ \psi_1(u)$ is the net leakage the physical significance of eq. /4a/ becomes quite simple: it is a balance equation for neutrons of lethargy u.

II.2. Approximations for $L_m(u)$

The elastic scattering transfer cross section $\Sigma^o(\mu_o,u)$ is a sum of analogous transfer cross sections for all isotopes present in the slab investigated:

$$\Sigma^o(\mu_o,u) = \sum_k \Sigma_k^o(\mu_o,u) \qquad /11/$$

where $\Sigma_k^o(\mu_o,u)$ is the elastic scattering transfer cross section for the k^{th} isotope. Accordingly, the elastic slowing down source $L_m(u)$ can be represented as a similar sum:

$$L_m(u) = \sum_k L_{mk}(u) \qquad /12a/$$

where

$$L_{mk}(u) = 2\pi \int_{-1}^{1} \psi_m(u')\ P_m(\mu_o)\ \Sigma_k^o(\mu_o,u')\ d\mu_o \quad . \qquad /12b/$$

In the remainder of this section, one isotope will be always concerned and, for the sake of simplicity, its subscript k will be omitted. In later sections this subscript will be taken up again.

First, the quantity $q_m(u)$ is introduced which vanishes at lethargies $u < 0$ and satisfies the equation

$$L_m(u) = \psi_m(u)\ G_m^o(u) - \frac{dq_m(u)}{du} \qquad /13/$$

where $G_m^n(u)$ is defined as

$$G_m^n(u') = \frac{2\pi}{n!} \int_{-1}^{1} P_m(\mu_o)(u'-u)^n\ \Sigma^o(\mu_o,u')\ d\mu_o \quad . \qquad /14/$$

Some of the coefficients G_m^n can be given a simple physical significane, e.g.

$$G_o^o(u') = 2\pi \int_{-1}^{1} \Sigma^o(\mu_o,u')\ d\mu_o = \Sigma^s(u') \qquad /15a/$$

is the elastic scattering cross section and

$$G_o^1(u') = 2\pi \int_{-1}^{1} \Sigma^o(\mu_o,u')(u'-u)\ d\mu_o = -\xi\Sigma^s(u') \qquad /15b/$$

where ξ is the average lethargy gain per elastic scattering collision.

Furthermore,

$$G_1^o(u') = 2\pi \int_{-1}^{1} \mu_o \, \Sigma^o(\mu_o, u') \, d\mu_o = \overline{\cos\theta_o} \, \Sigma^s(u') \qquad /15c/$$

where $\overline{\cos\theta_o}$ is the average cosine of the scattering angle in the laboratory system. Note finally that $q_o(u)$ is identical with the usual slowing down density.

For isotopes heavier than Al-27, the Fermi-age approximation is used in GRACE, i.e.

$$q_o(u) = \xi \, \Sigma^s(u) \, \psi_o(u) \quad , \qquad /16a/$$

$$q_1(u) \equiv 0 \quad . \qquad /16b/$$

For isotopes not heavier than Al-27, GRACE uses the Greuling-Goertzel approximation. It is described in detail in refs. [1] and [5], so that only the final equations are reproduced here. In this approximation, $q_m(u)$ satisfies the following equations:

$$q_o(u) + \lambda_o \frac{dq_o}{du} = -\psi_o \, G_o^1 \left(1 - \frac{d\lambda_o}{du}\right) \quad , \qquad /17a/$$

$$q_1(u) + \lambda_1 \frac{dq_1}{du} = -\psi_1 \, G_1^1 \left(1 - \frac{d\lambda_1}{du}\right) \qquad /17b/$$

where

$$\lambda_m = -\frac{G_m^2}{G_m^1} \quad . \qquad /18/$$

Comparison of Eqs. /16a/, /17a/, and /15b/ shows that in the Fermi-age approximation, the terms $\lambda_o \frac{dq_o}{du}$ and $d\lambda_o/du$ are neglected. In GRACE, Eq. /17b/ for the anisotropic slowing down density $q_1(u)$ is used only for the three lightest isotopes: hydrogene, deuterium, and berillium.

According to the approximations described in this section, the following classification of isotopes will be used in later sections /cf. refs. [1] - [4]/:

- "Fermi elements" are those for which Eqs. /16/ hold; they will be identified in common by the subscript F.

- Greuling-Goertzel elements" or "f-elements" are those for which Eqs. /17/ hold; they will be identified by the subscript f.
- "h-elements" are those for which Eq. /17b/ is taken into account; they will be identified by the subscript h. Note that an h-element is always a Greuling-Goertzel element as well.

If an isotope is mentioned in general i.e. without reference to this classification it will have the subscript k. The isotopes "known" by GRACE are in Table 1.

II. 3. The multigroup equations

The final step in deriving the set of equations which is solved by GRACE is the introduction of the multigroup approximation. The group structure used in GRACE can be found in Table 2. Let the lethargy limits of the j^{th} group be u_{j-1} and u_j, its lethargy width $\Delta u_j = u_j - u_{j-1}$. The last energy group is always the thermal group. Denote its subscript by j_{th}. Then j_{th} is the total number of lethargy groups as well. /The lethargy limits of the thermal group are not fixed in contrast to the other groups./

Define the following quantities:

$$\phi_j = \int_{u_{j-1}}^{u_j} \psi_o(u)\, du \qquad /19/$$

/group flux/

$$J_j = -i \int_{u_{j-1}}^{u_j} \psi_1(u)\, du \qquad /20/$$

/group current/

$$S_j = \int_{u_{j-1}}^{u_j} S(u)\, du \qquad /21/$$

$$I_j = \int_{u_{j-1}}^{u_j} I(u)\, du \qquad /22/$$

$$h_j = h\left(B, \Sigma_j^T\right) \qquad /23/$$

Σ_j^T will be defined later, cf. Eq. /26/.

The following isotope dependent quantities are to be defined for each isotope k present in the slab:

$$q_{kj} = q_{ok}(u_j) \quad , \qquad /24/$$

$$p_{kj} = -iq_{1k}(u_j) \quad , \qquad /25/$$

$$\Sigma_{kj} = \frac{1}{\phi_j} \int_{u_{j-1}}^{u_j} \Sigma_k(u)\, \psi_o(u)\, du \qquad /26/$$

where Σ_k stands for any type of cross section for isotope k. In the following, if the subscript k will be omitted from a cross section, this means a sum for all isotopes present:

$$\Sigma_j = \sum_k \Sigma_{kj} \quad .$$

Furthermore,

$$\mu_{kj} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{G_{1k}^o(u)}{\Sigma_k^s(u)}\, du \quad , \qquad /27/$$

$$\xi_{kj} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{G_{ok}^1(u)}{\Sigma_k^s(u)}\, du \quad , \qquad /28/$$

$$\eta_{kj} = -\frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{G_{1k}^1(u)}{\Sigma_k^s(u)}\, du \quad , \qquad /29/$$

$$\Gamma_{kj} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \lambda_{ok}(u)\, du \quad , \qquad /30/$$

$$Z_{kj} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \lambda_{1k}(u)\, du \quad . \qquad /31/$$

Finally, define the total slowing down densities by the equations:

$$q_j = \sum_k q_{kj} \quad , \qquad /32/$$

$$p_j = \sum_k p_{kj} \quad . \qquad /33/$$

Now integrate Eqs. /4a/ and /4b/ over the interval (u_{j-1}, u_j) bearing in mind Eq. /13/ for $L_m(u)$. Then one gets that

$$\Sigma_j^T \phi_j = \Sigma_j^s \phi_j + q_{j-1} - q_j - BJ_j + S_j + J_j \qquad /34a/$$

and

$$h_j \Sigma_j^T J_j = J_j \sum_k \Sigma_{jk}^s \mu_{jk} + p_{j-1} - p_j + \frac{B}{3} \phi_j \qquad /34b/$$

Eq. /17a/ holds for each of the f-elements. Its integration gives:

$$\frac{\Delta u_j}{2} \left(q_{fj} + q_{f,j-1}\right) + \Gamma_{fj}\left(q_{fj} - q_{f,j-1}\right) = \xi_{fj} \Sigma_{fj}^s \phi_j \left(1 - \frac{\lambda_{of}(u_j) - \lambda_{of}(u_{j-1})}{\Delta u_j}\right)$$

/35a/

A similar equation can be obtained for all h-elements from Eq. /17b/:

$$\frac{\Delta u_j}{2} \left(p_{hj} + p_{hj-1}\right) + Z_{hj} \left(p_{hj} - p_{h,j-1}\right) = \eta_{hj} \Sigma_{hj}^s J_j \left(1 - \frac{\lambda_{1h}(u_j) - \lambda_{1h}(u_{j-1})}{\Delta u_j}\right)$$

/35b/

If the sum of $q_{ok}(u)$ for all Fermi-elements is denoted by $q_F(u)$ the sum of Eq. /16a/ for all Fermi-elements yields:

$$q_{Fj} = \phi \sum_{k \epsilon F} \xi_{kj} \Sigma_{kj}^s \frac{1}{\Delta u_j} \quad . \qquad /36/$$

In order to simplify these equations to some extent, new notations are introduced. If N_k denotes the nuclear density of isotope k, define

$$\mu_{kj}\ \Sigma^{s}_{kj} = N_k\ M_{kj} \quad , \qquad /37/$$

$$\xi_{kj}\ \Sigma^{s}_{kj} = N_k\ \Theta_{kj} \quad , \qquad /38/$$

$$\xi_{fj}\ \Sigma^{s}_{fj} \left(1 - \frac{\lambda_{of}(u_j) - \lambda_{of}(u_{j-1})}{\Delta u_j} \right) = N_f\ \Theta^{*}_{fj} \quad , \qquad /39/$$

$$\eta_{hj}\ \Sigma^{s}_{hj} \left(1 - \frac{\lambda_{1h}(u_j) - \lambda_{1h}(u_{j-1})}{\Delta u_j} \right) = N_h\ H_{hj} \quad . \qquad /40/$$

Introducing the quantities defined by Eqs. /37/ to /40/ into Eqs. /34/ to /36/ and rearranging terms in such a way that terms referring to group j stand on the left hand side and terms referring to group /j-1/ stand on the right hand side, one gets the following set of equations:

$$B J_j + \left(\Sigma^{A}_{j} + A_j\ \Sigma^{I}_{j} \right) \phi_j + q_j = S_j + I_j + q_{j-1} \quad , \qquad /41a/$$

$$- \frac{B}{3}\ \phi_j + \left(h_j\ \Sigma^{T}_{j} - \sum_k N_k\ M_{kj} \right) J_j + p_j = p_{j-1} \quad , \qquad /41b/$$

$$\left(\Gamma_{fj} + \frac{\Delta u_j}{2} \right) q_{fj} - N_f\ \Theta^{*}_{fj}\ \phi_j = \left(\Gamma_{fj} - \frac{\Delta u_j}{2} \right) q_{f,j-1} \quad , \qquad /41c/$$

$$q_{Fj} = \phi_j \sum_{k \in F} \frac{N_k\ \Theta_{kj}}{\Delta u_j} \quad , \qquad /41d/.$$

$$\left(z_{hj} + \frac{\Delta u_j}{2} \right) p_{hj} - N_h\ H_{hj}\ J_j = \left(z_{hj} - \frac{\Delta u_j}{2} \right) p_{h,j-1} \quad . \qquad /41e/$$

These are the basic multigroup equations which are actually solved by GRACE. Eqs. /41a/, /41b/ and /41d/ are to be taken only once while Eqs. /41c/ and /41e/ as many times as there are f- and h-elements present, respectively. In Eq. /41a/, the term $A_j\ \Sigma^{I}_{j}$ requires some explanation. In this equation, the term I_j does not contain the contribution of those inelastic scattering collisions which do not transfer the colliding neutron to an other group and this is taken into account by the factor A_j. Thus $A_j\ \Sigma^{I}_{j}\ \phi_j$ gives the number of neutrons which are removed from group j by inelastic scattering.

Eqs. /41a/ to /41e/ hold for the thermal group, too, but some care has to be taken in applying them to the thermal group. Eqs. /41c/ to /41e/ are to be left out and in Eqs. /41a/ and /41b/, $q_{j_{th}} = p_{j_{th}} = I_{j_{th}} = 0$. Similarly, in the first group $p_o = q_o = I_o = 0$.

The solution of this set of equations is quite simple because there is no up-scattering in the epithermal energy range. It starts at $j = 1$ and proceeds up to $j = j_{th}$. Imagine that the solution has reached some group j. Then one knows $q_{f,j-1}$, $p_{h,j-1}$, and $q_{F,j-1}$ for all values of f and h, and I_j can be calculated from the equation:

$$I_j = \sum_{j'=1}^{j-1} \Sigma_{j'}^{I}, \; a_{j',j} \; \phi_{j'} \qquad /42/$$

where $a_{j',j}$ is the probability that a neutron scattered inelastically in group j' is removed to group j. It can be very simply seen that ϕ_j and J_j satisfy the following set of equations:

$$\alpha_{11} \; \phi_j + \alpha_{12} \; J_j = \alpha_{13} \qquad /43a/$$

$$\alpha_{21} \; \phi_j + \alpha_{22} \; J_j = \alpha_{23} \qquad /43b/$$

where

$$\alpha_{11} = \Sigma_j^A + A_j \; \Sigma_j^I + \sum_f \frac{N_f \; \theta_{fj}^*}{\Gamma_{fj} + \frac{\Delta u_j}{2}} + \sum_{k \in F} \frac{N_k \; \theta_{kj}}{\Delta u_j} \; , \qquad /44a/$$

$$\alpha_{12} = B \; , \qquad /44b/$$

$$\alpha_{13} = S_j + I_j + q_{F,j-1} + \sum_f \frac{\Delta u_j}{\Gamma_{fj} + \frac{\Delta u_j}{2}} \; q_{f,j-1} \; , \qquad /44c/$$

$$\alpha_{21} = - \frac{|B|}{3} \qquad /44d/$$

$$\alpha_{22} = h_j \; \Sigma_j^T - \sum_k N_k \; M_{kj} + \sum_h \frac{N_h \; H_{hj}}{Z_{hj} + \frac{\Delta u_j}{2}} \; , \qquad /44e/$$

$$\alpha_{23} = \sum_h \frac{\Delta u_j}{Z_{hj} + \frac{\Delta u_j}{2}} \; p_{h,j-1} \; . \qquad /44f/$$

After determining ϕ_j and J_j from Eqs. /43/, the slowing down densities q_{fj}, q_{Fj}, and p_{hj} can be calculated from Eqs. /41c/, /41d/ and /41e/, respectively. Then the solution proceeds to the next group and the whole procedure is repeated for it.

The solution of Eqs. /41/ is the heart of the code GRACE. This is fitted into the framework of various calculations and iterations. In the next two sections, these will be described.

II.4. Core regions

One of the main roles of GRACE is to calculate group constants for few-group criticality codes. For this purpose the best value of the buckling B is that at which the slab is critical. In case of core regions GRACE carries out an interation for finding out this value of B. Of course, this interation is optional.

Prior to iteration, one must know whether a real or an imaginary buckling has to be searched. If the core composition is such that $k_\infty > 1$, it is sure that there is a finite slab thickness at which this given core composition is critical. In this case, the iteration searches a real buckling. If $k_\infty < 1$, no cosine solution exists for the given composition and an imaginary buckling has to be found. Thus, first of all, the buckling B is set equal to zero and Eqs. /41/ are solved, as it is described in the previous section. Fom the solution, k_∞ is calculated using Eq. /8/. k_∞ is in itself an interesting quantity but in GRACE it is used only to decide whether real or imaginary buckling exists. In case of real B, Eq. /10c/ applies for β and Eqs. /41/ hold while in case of an imaginary B, Eq. /10d/ applies for β and the sign of B has to be changed to minus in Eq. /41a/. What actually happens in GRACE is that the sign is made negative in the imaginary case and the absolute value is taken for B in Eq. /41b/. This change of sign may be proved strictly [3] but can be simply made plausible. The term BJ_j represents the leakage in the neutron balance. If $k_\infty > 1$, this may be positive but if $k_\infty < 1$, there is a deficit in the neutron balance which has to be compensated by a net in-leakage. That is why this term is negative in the latter case.

Once this decision has been made, the criticality search can be done. The user of the code is supposed to specify an initial value for B. As the first step of the iteration, Eqs. /41/ are solved for this value of the buckling and from the solution k_{eff} is calculated using Eq. /8/. If $k_{eff} \neq 1$, the buckling B is changed until $k_{eff} = 1$ is reached. The relevant formulae of the iteration are those of ref. [3]. Suppose that n steps of iteration have been completed yielding $k_{eff,n}$ and a current $J_{j,n}$. Then the new value B_{n+1} of the buckling is calculated from the following equation:

$$B^2_{n+1} = B^2_n \left(1 + \frac{1 - k_{eff,n}}{k_{eff,n} \cdot \log P_{NL,n}} \right) \qquad /45/$$

where P_{NL} is the non-leakage probability given by the equation

$$P_{NL,n} = 1 \pm B_n \sum_{j=1}^{j_{th}} J_{j,n} \quad . \qquad /46/$$

In this last equation, sign + stands for imaginary buckling while sign - for real buckling. Of course, the P_{NL} as given by Eq. /46/ has a real physical significance /as the non-leakage probability/ only for real buckling.

This iteration proved to converge very fast in practice. It is stopped

- when the inequality

$$\frac{|B_{n+1} - B_n|}{|B_{n+1}|} < \varepsilon \qquad /47/$$

is fulfilled where ε is specified in input,

- or when the number of iterations has reached a maximum number /specified in input/,

- or when B^2_{n+1} and/or $P_{NL,n}$ becomes negative in Eq. /45/. These last two cases indicate generally that something was not well specified in input e.g. the initial value of the buckling is too large. The second criterion may be used to omit the iteration: if the maximum number of iteration is chosen to be 1, Eqs. /41/ will be solved only once for the B specified in input and, consequently, all further results of the code correspond to this buckling.

II.5. Reflector regions

As pointed out at the beginning of Section II. the reflector can not be expected to have a space-independent neutron spectrum. For this reason, Eqs./41/ based on the trial function in Eq. /2/ can not be used in their original form. Ref. [3] suggests a synthetic treatment which modifies Eqs. /41 only slightly and can be expected to give acceptable group constants.

An artificial but space dependent neutron flux may be written in the following form:

$$\phi(\mu,u,x) = e^{-B(u)x}\ \psi(\mu,u)\ . \qquad /48/$$

It this trial function is inserted into Eq. /1/ then one gets instead of Eqs. /4/:

$$\Sigma^T(u)\ \psi_o(u) = L_o(u) + B(u)\ J(u) + I(u)\ , \qquad /49a/$$

$$\Sigma^T(u)\ h(u)\ J(u) = L_1(u) + \frac{B(u)}{3}\ \psi_o(u) \qquad /49b/$$

because, in this case, $\psi_1(u)$ is real so that $\psi_1(u) = J(u)$. the boundary of core and reflector the leakage from the core is $BJ_{core}(u)$. This is set equal to $B(u)\ J_{refl.}(u)$. If before the given reflector a core region has been investigated by the code the lethargy dependence of this leakage is known. Since in a reflector the fission source term $S(u)$ of Eq. /4a/ is zero, the leakage of the core normalized to unity may be denoted by $S(u)$:

$$S(u) = \frac{B\ J_{core}(u)}{\int_0^\infty B\ J_{core}(u)\ du}\ . \qquad /50/$$

This is not merely a question of notation but it facilitates the formulation of the equations. Now Eqs. /49a/ and /49b/ can be written as

$$\Sigma^T(u)\ \psi_o(u) = L_o(u) + S(u) + I(u)\ , \qquad /51a/$$

$$\Sigma^T(u)\ h(u)\ J(u) = L_1(u) + \frac{B(u)\ \psi_o(u)}{3} \qquad /51b/$$

and one has the additional equation

$$B(u)\ J(u) = S(u)\ . \qquad /51c/$$

If the Greuling-Goertzel and multigroup approximations are introduced again in Eqs. /51/ almost the same equations result as Eqs. /41/. The only modifications are that the buckling is group dependent and Eq. /41a/ now reads as

$$\left(\Sigma_j^A + \Lambda_j\ \Sigma_j^I\right)\phi_j + q_j = S_j + I_j + q_{j-1}\ . \qquad /52a/$$

The multigroup form of Eq. /51c/ is clearly

$$B_j J_j = S_j \quad . \qquad /52b/$$

As a consequence of these modifications, Eq. /43a/ does not contain J_j since it is missing from Eq. /52a/. One now has

$$\alpha_{11} \phi_j = \alpha_{12} \qquad /53/$$

or

$$\phi_j = \frac{\alpha_{12}}{\alpha_{11}} \qquad /54/$$

where the coefficients α have been defined by Eqs. /44/. The second equation /i.e. Eq. /43b// is used to determine the group buckling B_j. From Eq. /52b/, J_j can be expressed as

$$J_j = \frac{S_j}{B_j} \qquad /55/$$

which inserted into Eq. /43b/ leads to an algebraic equation of second order for B_j:

$$B_j^2 \frac{\phi_j}{3} + B_j \alpha_{23} - \alpha_{22} S_j = 0 \qquad /56/$$

since $\alpha_{21} = - \frac{B_j}{3}$ /cf. Eq. /44d//. B_j is the positive root of Eq. /56/:

$$B_j = \frac{-\alpha_{23} + \sqrt{\alpha_{23}^2 + \frac{4}{3} \phi_j \alpha_{22} S_j}}{\frac{2}{3} \phi_j} \quad . \qquad /57/$$

Once B_j is known, J_j can be obtained from Eq. /55/. This completes the solution of the set of equations consisting of Eqs. /52a/, /52b/, and /41b/ to /41e/. It must be added that when using the B_1 approximation, α_{22} depends on B_j through h_j as it can be seen from Eqs. /44e/, /10b/, and /10d/. In this case, solution of Eqs. /56/ requires a simple iteration for all values of j.

As a matter of fact, the best agreement with experimental results has been obtained when the P_1 approximation was used for reflectors.

II.6. Microgroup constants

The multigroup equations solved by GRACE contain material constants defined in Section II.3. They are stored in the 40 group GRACE library for the isotopes listed in Table 1. For cross sections which are smooth over a GRACE group, Eq. /26/ can be approximated as

$$\Sigma_{kj} \approx \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \Sigma_k(u)\, du = N_k\, \sigma_{kj} \quad . \qquad /58/$$

For groups in which cross sections are smooth these averages σ_{kj} are stored in the library.

In case of resonance materials, however, the approximation made in Eq. /58/ can not be tolerated in those groups which contain resonances. For such resonance groups the flux weighted average in Eq. /26/ depends on the presence of other isotopes and of lattice effects.

There is another energy range in which the presence of other isotopes and lattice structure influence the group constants of a given isotope: this is the thermal energy range.

Now for isotopes having smooth cross sections in the epithermal energy range, macroscopic cross sections are calculated by multiplying the nuclear density of the given isotope by the microscopic group constants found in the GRACE library. The same applies for resonance isotopes, too, in groups not containing resonances.

Resonance absorption and fission can be taken into account in GRACE in two different ways.

II.6.a. RIFFRAFF type resonance treatment

The simplest way to treat resonances is to calculate directy, for the given composition and lattice, the flux $\phi(\underline{r},u)$ as a function of space and energy inside the elementary cell and then to form following averages:

$$\sigma_{kj} = \frac{\int_{V_{cell}} \int_{u_{j-1}}^{u_j} \Sigma_k(\underline{r},u)\, \phi(\underline{r},u)\, du\, d\underline{r}}{\overline{N}_k \int_{V_{cell}} \int_{u_{j-1}}^{u_j} \phi(\underline{r},u)\, du\, d\underline{r}} \qquad /59/$$

where $\bar{N}_k$ is the homogenized nuclear density of isotope k. For homogeneous cores, of course, space averaging disappears.

Averages of the type of Eq. /59/ have to be calculated by separate codes. For two region cylindrical cells, this can be done by the code RIFFRAFF, for homogeneous systems by the code RA04 [6]. If this resonance option is used in GRACE, averages of the absorption, fission and scattering cross sections as expressed by Eq. /59/ have to be provided in input for all resonance elements present in the system and for all of their resonance groups. Table 3. shows those elements which are considered in GRACE as resonance elements together with indication of their resonance groups.

These input cross sections are then used in GRACE as if they would have been taken from the library. For both resonance and non-resonance groups, Eqs. /41/ apply when using this resonance option.

II.6.b. BIGG type resonance treatment

Another treatment of resonance absorption and fission is described in refs. [2] and [3] which involves some modifications of the set of equations /41/ but requires a simpler input preparation. This treatment is based on semi-empirical effective resonance integrals. The main ideas and the relevant formulae are the following.

An effective resonance integral for a given resonance is defined as a resonance integral which multiplied by a fictitious flux or the so-called "switch off flux" gives the reaction rate per absorbing atom for the given resonance. The expression "switch off flux" means the flux which would exist in the absence of the resonance.

Resonance integral for a GRACE microgroup can be considered as a resonance integral for a resonance peak, because the microgroup structure of GRACE is such that generally one big resonance peak and several small peaks fall into one microgroup. GRACE is based on the semi-empirical formulae of Hellstrand /cf. Section II.7./ which give single pin resonance integrals for the whole energy range: R_{SP}. The lattice resonance integrals R_L for the resonance energy range are obtained from the equation

$$R_L = \alpha \left(R_{SP} - R_{SP}^H \right) \qquad /60/$$

where R_{SP}^H is the high energy contribution to the single pin value and α is the mutual shielding factor of the fuel pins in the lattice. This lattice integral R_L is then distributed among the different resonance groups by

multiplying it by a distribution function ψ_j normalized to unity:

$$\Delta R_j = \psi_j R_L \qquad /61/$$

where

$$\sum_{j=1}^{j_{th}} \psi_j = 1 \quad . \qquad /62/$$

The fictitious flux is calculated as follows. If the resonance is switched off, the absorption cross section can be neglected with respect to the scattering cross section and then Eq. /4a/ may be written in the following form:

$$\Sigma^s(u)\, \phi_o(u) = L_o(u) - BJ_o(u) \qquad /63/$$

where subscript O at ϕ and J indicates that the solutions of Eq. /63/ are the fictitious flux and current. At the moment when the resonance absorption in group j is calculated, the flux and current for groups 1,2,..., /j-1/ are known. For this reason, $L_o(u_{j-1})$ can be calculated. An approximate expression for it is given in ref. [2]/:

$$L_o(u_{j-1}) = \sum_k \frac{1}{1-\alpha_k} \sum_i \Sigma^s_{ki} \frac{\phi_i}{\Delta u_i} \int_{\Delta u_i} e^{-(u_{j-1}-u)}\, du \qquad /64/$$

where

$$\alpha_k = \left(\frac{A_k - 1}{A_k + 1} \right)^2$$

for element k with mass number A_k and summation for i starts from the microgroup containing the lethargy value $(u_{j-1} + \log\alpha_k)$ and ends at group /j-1/. A heuristic interpretation of expression /64/ may be given as follows: $\Sigma^s_{ki}\, \phi_i/\Delta u_i$ is the average scattering rate in microgroup i by element k and

$$\frac{1}{1 - \alpha_k} \int_{\Delta u_i} e^{-(u_{j-1}-u)}\, du\, du'$$

is the probability of transfer from group i to a lethargy in the interval du' at u_{j-1}. The expression /64/ sums up the contributions of all elements

and lethargy groups.

Furthermore, if there is no resonance absorption, it may be assumed that the flux and current in group j are equal to the flux and current at the lethargy u_{j-1}. $J_o(u_{j-1})$ is further approximated by the average current in microgroup /j-1/ i.e.

$$J_o(u_{j-1}) \approx \frac{J_{j-1}}{\Delta u_{j-1}} \quad .$$

Then Eq. /63/ may be rewritten as

$$\Sigma^s(u_{j-1})\ \phi_o(u_{j-1}) \approx L_o(u_{j-1}) - BJ_{j-1}/\Delta u_{j-1}$$

which gives the fictitious flux ϕ_{oj} for the resonances in group j:

$$\phi_{oj} \approx \frac{1}{\Sigma^s_{j-1}} \left[L_o(u_{j-1}) - B \frac{J_{j-1}}{\Delta u_{j-1}} \right] \quad . \qquad /65/$$

Now, according to the definition of the effective resonance integrals, the absorption rate in group j is given by the equation

$$(RA)_j = \sum_k N_k\ \Delta R_{kj}\ \phi_{oj} \qquad /66/$$

In ref. [3], a better approximation is suggested for the reaction rate $(RA)_j$ instead of Eq. /66/. This reads as

$$(RA)_j = q_{j-1}\left(1 - P_j\right) \qquad /67/$$

where P_j is the resonance escape probability for microgroup j. It is shown [3] that a good approximation for P_j is

$$P_j = \exp\left\{ - \frac{\phi_{oj}}{q_{j-1}} \sum_k N_k\ \Delta R_{kj} \right\} \quad . \qquad /68/$$

If reaction rates for a given isotope are needed in microgroup j, this can be obtained approximately from the formula

$$(RZ)_{kj} = \frac{N_k \, \Delta R^z_{kj}}{\sum_{k'} N_{k'} \, \Delta R_{k'j}} \, (RA)_j \qquad /69/$$

where superscript z may indicate capture or fission.

Finally, it must be noted that when integrating Eq. /4b/ for the interval Δu_j /in order to get the multigroup equations/ averages of the type

$$\Sigma'_{kj} = \frac{1}{J_j} \int_{u_{j-1}}^{u_j} \Sigma_k(u) \, J(u) \, du \qquad /70/$$

ought to have been introduced instead of averages defined by Eq. /26/. So far these averages have been tacitly approximated as

$$\Sigma'_{kj} = \frac{1}{J_j} \int_{u_{j-1}}^{u_j} \Sigma_k(u) \, \psi_o(u) \, \frac{J(u)}{\psi_o(u)} \, du \approx \frac{1}{\phi_j} \int_{u_{j-1}}^{u_j} \Sigma_k(u) \, \psi_o(u) \, du = \Sigma_{kj} \qquad /71/$$

The adequacy of this approximation is proved only by practice. In order to remain at the same level of approximation, the best way of treating resonances in Eq. /4b/ is the approximation

$$\sum_k N_k \int_{u_{j-1}}^{u_j} \sigma_k(u) \, J(u) \, du \approx q_{j-1} \left(1 - P_j\right) \frac{J_{j-1}}{\phi_{j-1}} \, . \qquad /72/$$

Now when using the BIGG-type resonance option, Eqs. /41a/ and /41b/ are modified to

$$BJ_j + \left(\Sigma^A_j + A_j \, \Sigma^I_j\right) \phi_j + q_j = S_j + I_j + q_{j-1} - q_{j-1} \left(1 - P_j\right) \qquad /73a/$$

$$-\frac{B}{3} \phi_j + \left(h_j \, \Sigma^T_j - \sum_k N_k \, M_{kj}\right) J_j + p_j = p_{j-1} - h_j \, q_{j-1} \left(1 - P_j\right) \frac{J_{j-1}}{\phi_{j-1}} \qquad /73b/$$

where Σ^A_j and Σ^T_j contain only the contributions of smooth cross sections.

II.6.c. Thermal group constants

Beside the resonance region, the other energy range in which spectrum variation inside a GRACE microgroup and lattice effects are important is the thermal energy range. These effects are not taken into account by GRACE. Therefore, a separate code is needed calculating the same cell average as expressed by Eq. /59/ for the thermal energy range. This can be done e.g. by THERMOS. Of course, for a given value of the buckling B the fast spectrum is completely independent of the thermal group. This means that if no buckling iteration /cf. Section II.4./ is required and only the fast neutron spectrum needs be calculated the values of the thermal group constants are irrelevant.

Thus, the following quantities are to be supplied in input: $\Sigma^A_{j_{th}}$, $\Sigma^s_{j_{th}}$, $\left(\nu\Sigma^F\right)_{j_{th}}$, $M_{j_{th}}$ $\left(= \Sigma^s_{j_{th}} \overline{\cos\theta_o}\right)$. Note that these macroscopic cross sections contain the contributions of all isotopes present in the cell.

In connection with the thermal group, a further information must be given in input: its energy limits. For this purpose it is enough to specify the value of j_{th} because GRACE makes a single group from all microgroups numbered by j_{th}, $j_{th}+1,\ldots,40$ in Table 2. A proper choice of j_{th} can assure that there should be no up-scattering from the thermal group.

It must be mentioned here that, independently from the foregoing equations, further thermal data are required in case of core regions. These are macroscopic cell averaged thermal absorption and fission cross sections for each fissionable and fertile isotopes present in the cell. This information will be needed in the calculation of spectrum indices /see Section III./.

II.7. The DATAPREP subroutine

A special subroutine is included in GRACE in order to facilitate input preparation. This is based on formulae of ref. [4] so that they are not reproduced here. The functions of subroutine DATAPREP are:

- From cell data and material densities /which are given in g/cm^3/ it calculates homogenized nuclear densities. The lattice may be triangular or square, the cell may be composed from a fuel rod, a clad surrounded by moderator.
- It calculates a fast advantage factor which takes into account that at high energies the flux is peaked in the fuel rod owing to the fission source inside it. Cross sections of isotopes not lighter than Th-232 are multiplied by this factor in the highest

7 microgroups /cf. Table 2./.

- Finally, subroutine DATAPREP calculates the single pin resonance integrals and mutual shielding factors needed by the BIGG-type resonance treatment /see Section II.6.b./ for the fuel temperature specified in input. This latter function of the subroutine is optional i.e. if the user has his own resonance integrals and mutual shielding factors he may give them in input and the code will use them. It should be noted that the subroutine calculates resonance data for U-235 and U-238 in the form of uranium metal or UO_2; for the other isotopes, resonance data have to be specified by the user.

The use of subroutine DATAPREP is optional. If it is not used /e.g. for reflector regions, this must always be the case/, then homogenized nuclear densities, the fast advantage factor, and single pin resonance integrals and mutual shielding factors /if there are any resonance isotopes/ have to be specified in input.

III. User's manual

III.1. Input preparation

The input subroutine of GRACE has been written in such a way that the input preparation requires only data which are always available for a reactor composition and necessitates a minimum of preliminary calculations to be carried out by hand. The overall organization of the code permits to solve any number of problems one after the other. The only restriction is that the first problem has to deal with a core region because the source for a reflector region is calculated using the leakage from the region previously treated. It should be noted that if several reflector regions follow each other the spectrum of their source will be identical. This is a direct consequence of the energy dependent buckling approximation.

In the following, a detailed description of the input preparation will be given. Input data are to be punched on paper tape. But in order to make understanding of the rules of input preparation easier, the expression "card" will be used for one record /i.e. one line/ of the paper tape. The format of each card will be given in FORTRAN notation.

1st card /10A8/: The problem is given a title the length of which may not exceed 80 characters.

2nd card /4L4, 2I4, E4.0,I4, 2E8.4,7I4/: This card contains the most important control variables of the problem.

char. 1 to 4: Punch T /=True/ for P_1 approximation and F /=False/ for B_1 approximation.

char. 5 to 8: If the RIFFRAFF-type resonance treatment is used, punch T while for the BIGG-type treatment punch F.

char. 9 to 12: If T is punched the code will compute few-group constants <u>also</u> for the infinite medium spectrum. For F this is not done.

N.B. In case of reflectors it is immaterial what is punched in these last two fields.

char. 13 to 16: This field controls the output. For T , detailed slowing down densities will be printed out in the output for all elements while, for F, this will be left out.

char. 17 to 20: The value of this variable /NHOM/ controls the lattice homogenization /cf. Section II.7./. If it is

0: the case of no homogenization;

1: the code does the lattice homogenization and calculates resonance integrals and mutual shielding factors using semi-empirical formulae;

2: the code does lattice homogenization without calculating the resonance data. In this case, these latter must be supplied by the user.

N.B. If the RIFFRAFF option in used, only 0 or 2 are acceptable. Furthermore, for reflectors a 0 must always be punched.

char.21 to 24: For a core region punch 1, for a reflector punch 4.

char.25 to 28: For value of ε mentioned in Section II.4. /Usually $\varepsilon = 10^{-5}$/.

char.29 to 32: The maximum number of iterations. Generally, it must be a positive integer. If it is -1 calculations will be done only for the infinite medium /in case of core regions/.

char. 33 to 40: This field contains the buckling B in cm^{-1}. This B will be the starting value of the buckling iteration.

N.B. For reflector regions this value is not used. It must not be zero nor negative for core regions. /The code corrects for such input errors./ Practice has shown that the buckling iteration by Eq. /45/ may diverge if too large a starting B is used.

char. 41 to 48: The fast advantage factor.

N.B. Its value has to be specified only for core regions and only if NHOM=0 was punched in char. 17 to 20.

char. 49 to 52: The number of macrogroups in the calculation of few-group diffusion constants. It may be any integer number between 1 and 6.

char. 53 to 56: The highest microgroup index of the first macrogroup /cf. Table 2/. In other words, this specifies the lower energy limit of the macrogroup.

char. 57 to 60: The highest microgroup index of the second macrogroup.

and so on for each of the macrogroups.

N.B. As it was pointed out in Section II.6.c. the microgroup index j_{th} of the thermal group is given in input. Now j_{th} is the last macrogroup boundary. Thus, strictly speaking, the definition of the last macrogroup boundary is somewhat different from the definition of the other ones. If one-group constants are needed punch nothing else than j_{th} in char. 53 to 56.

The subsequent cards depend on what was specified for NHOM. For this reason two cases must be distinguished: a/ when the code does homogenization /NHOM = 1 or 2/ and b/ when it does not /NHOM = 0/.

a/ <u>No homogenization</u>

If the user supplies homogenized nuclear densities /what is always the case for reflectors/ the third and subsequent cards contain information concerning the elements present in the system under investigation. The format of each card is: /A8, 3E8.4,I2, 2E8.4,I2/. For each element it is specified:

char. 1 to 8: The identification symbol of the element which must be exactly the same as given in Table 1. No space should be punched in front of the element identification.

char. 9 to 16: Homogenized nuclear density of the element in units of $10^{24}/cm^3$.

char. 17 to 24: Single pin absorption resonance integral for the total energy range in barn.

char. 25 to 32: Mutual shielding factor for absorption.

char. 33 to 34: The index of the absorption ψ function /cf. Eqs. /61/ and /62// to be used for the element. The total number of ψ functions available for the various resonance elements is given in Table 3.

char. 35 to 42: Single pin fission resonance integral for the total energy range in barns.

char. 43 to 50: Mutual shielding factor for fission.

char. 51 to 52: The index of the fission ψ function to be used for the element.

Some important remarks have to be made concerning these element cards:

- The elements must be punched in the same order as they are listed in Table 1.
- The sequence of the element cards is finished by a blank card if this problem will be followed by other ones. If this problem is to be the last one punch the characters END in the first three positions of the finishing card and leave blank the rest of it.
- The maximum number of elements permitted in one problem is 18.
- The number of Greuling-Goertzel elements /cf. Section II.2./ may not be zero and may not exceed 8.
- The maximum number of Fermi-elements permitted in one problem is 10 when the RIFFRAFF resonance option is used.
- Only resonance elements may follow the first resonance element. GRACE considers an element to be a resonance element if the single pin resonance integrals are different from zero. /If NHOM = 1 or 2 the indices of the ψ functions are used for the same purpose./ A fertile element is defined as a resonance element for which the fission resonance integral is zero. The maximum number of resonance elements is 7, and 4 of them may have resonance fission.
- If the BIGG-type resonance option is used the indices of the ψ-functions may not be zero for resonance elements.

b/ Homogenization

If the lattice is homogenized by the code /NHOM = 1 or 2/ the third card contains generalities about the fuel lattice. Its format is /A8, 6E8.4/:

3rd card

char. 1 to 8: Type of the lattice. For a square lattice punch the characters SQUARE, for a triangular lattice punch the characters TRIANGLE. Nothing else is accepted.

char. 9 to 16: Lattice pitch in cm.

char. 17 to 24: Radius of the fuel rod /without clad!/ in cm.

char. 25 to 32: Thickness of the clad in cm. If there is no clad punch zero.

char. 33 to 40: Fuel temperature in K^{o}.

char. 41 to 48: Moderator temperature in K^{o}. If a zero is punched for it the code puts it equal to the fuel temperature.

char. 49 to 56: Enrichment of the fuel. If it is given in atom % punch it with a positive sign while a negative sign means an enrichment given in w/o. Of course, if the fuel is not uranium or if the densities of the individual uranium isotopes are known for the user the fuel enrichment need to be specified.

The 4th and subsequent cards contain element data. Their format is /A8, 1X,E8.4,2I2,4E8.4/.

char. 1 to 9: The identification symbol of the element.

char. 10 to 17: Density of the element in g/cm^3.

char. 18 to 19: Index of the ψ function for absorption /see Table 3/.

char. 20 to 21: Index of the ψ function for fission.

char. 22 to 29: Single pin absorption resonance integral for the total energy range.

char. 30 to 37: Mutual shielding factor for absorption.

char. 38 to 45: Single pin fission resonance integral for the total energy range.

char. 46 to 53: Mutual shielding factor factor for fission.

The following rules apply to the preparation of these element cards:

- The cell homogenization may be required from the code only for triangular or square lattices and the use of the semi-empirical formulae of resonance data only for UO_2 or uranium metal.
- As element identifications, the symbols listed in Table 1 may be used. Besides them some others are also accepted by the code. If the fuel is UO_2 punch OXIDE, if it is uranium metal punch METAL. If the cell contains water the symbol H2O may be used. When using any of these symbols, of course, the density of the oxide, metal or water is given in char. 10 to 17. If NHOM = 1 was punched on the 2nd card one of the symbols OXIDE or METAL must be used while for NHOM = 2 their use is not compulsory.
- If the symbols OXIDE or METAL are used they must be punched on the 4th card /i.e. the first element card/. Resonance data on this card refer to U-235. The resonance data for U-238 are given on the next card. Of course, positions 1 to 17 may be left blank on this card.
- The elements present in the fuel are punched first. The sequence of fuel cards is finished by a card containing the symbol CLAD in the first five positions. After this card follow the clad elements. Their sequence is finished by a card containing the symbol MODERATOR

in the first nine positions. After this card follow the moderator elements. Their sequence is finished by a blank card if this problem is followed by other ones while by a card containing the symbol END in the first three positions if this is the last problem. If there is no clad the sequence of fuel cards is finished by the symbol MODERATOR and clad is not mentioned at all.

- Apart from the above restrictions the order of the non-resonance elements is arbitrary. As to resonance elements, their order must correspond to the order in Table 1. As a consequence of this, Th-232 and U-233 may not be present if the symbols OXIDE or METAL are used. Any non-resonance element may be mentioned several times.
- The maximum number of element cards is 54. /The symbols OXIDE, METAL, and H2O are equivalent to 3,2, and 2 cards, respectively./ The same restrictions apply to the maximum number of elements in the cell as in the case of no homogenization /i.e. 8 f-elements, 10 Fermi-elements when using the RIFFRAFF-type resonance option, all elements: 18/.
- An element is considered to be a resonance element if the indices of the ψ functions are different from zero /the single pin resonance integrals are used for the same purpose if NHOM = 0/. For a fertile element the index of the ψ function for fission is zero.
- The indices of the ψ functions must be given for all resonance elements even when NHOM = 1 /i.e. when resonance integrals and mutual shielding factors are calculated by the code/. If NHOM = 2 and the BIGG-type resonance option is used, all resonance data have to be specified for all resonance elements.

RIFFRAFF input

In case of the Bigg-type resonance option, all resonance data have been given on the element cards but not so if the RIFFRAFF option is used. Therefore the blank or the "END" card finishing the sequence of the element card is followed by the homogenized microgroup constants for the resonance groups when the RIFFRAFF option is used. In connection with the element cards, it was explained how an element is declared to be a resonance element. Although resonance itegrals and ψ functions are not necessary when using the RIFFRAFF-type resonance treatment some arbitrary non-zero value must still be punched for them only to indicate the resonance character of the element.

First RIFFRAFF card /I2/: in characters 1 to 2 is punched the number of those elements for which RIFFRAFF input is given. This number must be equal to the number of resonance absorption elements.

The next cards are to be punched for all RIFFRAFF elements.

Identification card /A8,I3/:

char. 1 to 8: identification symbol of the element.

char. 9 to 11: number of resonance groups for which RIFFRAFF cross sections will be punched. This card is followed by the

Resonance group cards /I3,3E12.6/ the number of which must be equal to the number punched on the identification card.

char. 1 to 3: index of the GRACE microgroup for which homogenized cross sections are given on this card;

char. 4 to 15: absorption cross section in barns;

char. 16 to 27: fission cross section in barns;

char. 28 to 39: scattering cross section in barns.

N.B. The order of RIFFRAFF elements must be the same as that of the resonance elements in Table 1. For a given element, the micro-group having the smallest index should be punched first. Otherwise the order of microgroups is arbitrary.

Thermal data

The last cards contain cross sections for the thermal group /cf. Section II.6.c./. They follow the RIFFRAFF cards or, when the BIGG-type resonance option is used, the blank or the "END" card. The format of each thermal card is /7E8.4/.

1st Thermal card: macroscopic cross sections in cm^{-1}.

char. 1 to 8: $\Sigma^A_{j_{th}}$

char. 9 to 16: $\Sigma^s_{j_{th}}$

char. 17 to 24: $M_{j_{th}}$

char. 25 to 32: $(\nu\Sigma^F)_{j_{th}}$

For reflector regions this card completes the input of a problem. In case of core regions, two more cards are punched:

2nd Thermal card:

char. 1 to 8: contribution of the first resonance element to $\Sigma^{A}_{j_{th}}$ in cm^{-1};

char. 9 to 16: contribution of the second resonance element to $\Sigma^{A}_{j_{th}}$ in cm^{-1};

etc.

3rd Thermal card: contributions of all resonance fission elements to $\Sigma^{F}_{j_{th}}$ /not to $(\nu\Sigma^{F})_{j_{th}}$!/ punched in the same way as on the 2nd thermal card. /Only fissionable elements are mentioned on this card./

N.B. The thermal absorption and fission cross sections of any resonance element may not be punched to be the same because the code divides by their difference.

Finally, it is noted that the input subroutines of GRACE check the input data in order to prevent execution errors in the course of the calculations. If mistakes are discovered in the input the code prints out an error message and turns to the next problem. Of course, the code is not protected against all possible input errors but only the most commonly encountered ones.

III.2. Output description

The output of GRACE is self-explanatory for those who are familiar with its algorithm. Therefore, a brief summary of output results is sufficient.

First, all input data are reproduced in the output. The code does this before solving the slowing down equations. Thus the user has this even if the code finds some errors in the input data. In case of a detected input mistake, the code output is finished by the error message indicating the nature of the mistake.

Next follow the results of the iteration. For core regions, they are introduced by the value of the infinite multiplication factor and, optionally, few-group diffusion constants, etc. /see later/ for the infinite medium spectrum. For each step of the iteration the code prints out: buckling B, k_{eff}, P_{NL} /cf. Eq. /46//, fractional change of B. For reflector regions, there is no iteration unless B_1 approximation is used. Therefore only some final results are printed: the total number of iterations /if any/, average value $\bar{B}$ of the B_j's, and

$$\frac{\max(B_j) - \min(B_j)}{\bar{B}}$$

Then the most important results of GRACE are printed: the few-group diffusion constants. These are:
Group flux:

$$\phi_M = \sum_{j \in M} \phi_j \qquad /74/$$

where summation for j goes for microgroups in macrogroup M.
Group leakage:

$$Y_M = \sum_{j \in M} B_j J_j \qquad /75/$$

Macrogroup cross sections for absorption:

$$\Sigma_{aM} = \frac{\sum_{j \in M} \Sigma_j^A \phi_j}{\phi_M} \qquad /76/$$

and for fission

$$\left(\nu\Sigma_f\right)_M = \frac{\sum_{j \in M} \left(\nu\Sigma^F\right)_j \phi_j}{\phi_M} \qquad /77/$$

Of course, in case of the BIGG-type resonance treatment, the contributions of resonance absorption and fission in Eqs. /76/ and /77/ are taken into account according to Section II.6.b.
Diffusion constant:

$$D_M = \frac{Y_M}{\sum_{j \in M} B_j^2 \phi_j} \qquad /78/$$

Fission spectrum:

$$\chi_M = \sum_{j \in M} S_j \qquad /79/$$

Removal cross section:

$$\Sigma_{RM} = \frac{Q_M^R + I_M^R}{\phi_M} \qquad /80/$$

where Q_M^R and I_M^R are the removal rates from macrogroup M by elastic and inelastic scattering, respectively.
Energy exchange matrix:

$$f_{M' \to M} = \frac{Q_{M' \to M} + I_{M' \to M}}{\phi_{M'} \Sigma_{RM'}} \qquad /81/$$

where $Q_{M' \to M}$ and $I_{M' \to M}$ are removal rates from macrogroup M' to macrogroup M by elastic and inelastic scattering, respectively. The calculation of these removal rates is detailed in Appendix A.

Finally, effective cross sections are printed out for a 1/v cross section:

$$\Sigma_M^{1/v} = \frac{\sum_{j \in M} 1/v_j \ \phi_j}{\phi_M} \qquad /82/$$

where v_j is substituted in cm/sec i.e.

$$\frac{1}{v_j} = \frac{1.451.10^{-6}}{\Delta u_j} \left(\frac{1}{\sqrt{E_j}} - \frac{1}{\sqrt{E_{j-1}}} \right) \qquad /83/$$

because E is measured in eV.

Beside macrogroup constants, GRACE prints out the following microgroup data: ϕ_j, J_j, B_j, absorption rate, production rate, leakage rate, total slowing down density. At the user's option, all elementwise slowing down densities are printed out as well.

For comparisons with experiments, the following integral spectral indices are also calculated based on fomulae of ref. [3]:

Resonance escape probability:

$$p = \frac{q_{j_{th}} - 1}{P_{NL}} \qquad /84/$$

Fast fission factor:

$$\varepsilon = \frac{k_{eff}}{\int_0^\infty \nu \Sigma^F_{fiss}(u) \ \phi(u) \ du} \qquad /85/$$

where Σ^F_{fiss} contains contributions only from resonance fission elements.

$$\text{Conversion ratio} = \frac{\text{capture in all fertile elements}}{\text{absorption in all fissile elements}}$$

Elementwise quantities:

$$\delta_{fert} = \frac{\text{fissions in the fertile element}}{\text{fissions in all fissile elements}}$$

$$\delta_{fiss} = \frac{\text{epithermal fissions in the fissile element}}{\text{thermal fissions in the fissile element}}$$

$$\rho_{fert} = \frac{\text{epithermal captures in the fertile element}}{\text{thermal captures in the fertile element}}$$

$$\rho_{fiss} = \frac{\text{epithermal captures in the fissile element}}{\text{thermal captures in the fissile element}}$$

III.3. Machine requirements

GRACE requires a memory capacity of 20700 words and a scratch magnetic tape on the ICT-1905 computer. This tape is needed because GRACE is an overlay program. In addition, a second magnetic tape desk is necessary for the cross section library. The output of the code for a problem is not more than 12 line printer pages.

The running time for a problem is rarely more than 2 minutes. For reflectors, it is about 1 minute.

References

/1/ O.P. Tverbakk, J.M. Dϕderlein, BIGG-I, A Multigroup Neutron Spectrum and Criticality Code, Kjeller Report KR-77 /1964/.

/2/ G.A.G. deCoulon, L.D.Gates, and W.R.Worley, SSCR Basic Physics Program - Theoretical Analysis, Part II. BPG Computer Program Report, BAW-1230 /1962/.

/3/ O.P. Tverbakk and J.M. Døderlein, BIGG-II, A Multigroup Neutron Spectrum and Criticality Code, Kjeller Report KR-75 /1965/.

/4/ R.J.J. Stamm'ler et al.,DATAPREP-II, A Reactor Lattice Homogenization and BIGG-II Data Preparation Computer Code, Kjeller Report KR-78 /1965/

/5/ Naval Reactor Physics Handbook, Vol. I. Editor: A. Radkowsky /1964/.

/6/ Z. Szatmáry and Anna Bagyinszki, Calculation of Resonance Integrals - Code RIFFRAFF and RA04, Report KFKI-12 /1970/, Budapest.

/7/ J. Valkó, RJT1 - THERMOS, to be published.

/8/ Z. Szatmáry and J. Vigassy, SISYPHUS - a Code for the Solution of Few-group Diffusion Equations in Two Dimensions, Report KFKI-13 /1970/, Budapest.

Table 1.

List of GRACE elements

1	H-1
2	H-2
3	BE-9
4	B-NAT
5	B-1O
6	C-12
7	Θ-16
8	AL-27
9	ST. STEEL
1O	ZIRCALΘY
11	CD-NAT
12	XE-135
13	SM-149
14	SM-151
15	BI-2O9
16	TH-232
17	U-233
18	U-235
19	U-238
2O	PU-239
21	PU-24O
22	PU-241
23	FISSIUM

Table 2.

Group structure of GRACE

1	$7{,}189.10^{6}$	0,33003	0,33003
2	$5{,}169.10^{6}$	0,65991	0,32988
3	$3{,}716.10^{6}$	0,98994	0,33003
4	$2{,}671.10^{6}$	1,32013	0,33019
5	$1{,}92.10^{6}$	1,65026	0,33013
6	$1{,}381.10^{6}$	1,97978	0,32952
7	$9{,}926.10^{5}$	2,31001	0,33023
8	$8{,}2085.10^{5}$	2,5	0,18999
9	$5{,}13.10^{5}$	2,97006	0,47006
10	$3{,}688.10^{5}$	3,30008	0,33002
11	$2{,}652.10^{5}$	3,62985	0,32977
12	$1{,}906.10^{5}$	3,96016	0,34031
13	$1{,}37.10^{5}$	4,29036	0,33020
14	$5{,}572.10^{4}$	5,19000	0,89964
15	$2{,}265.10^{4}$	6,09018	0,90018
16	$9{,}21.10^{3}$	6,99005	0,89987
17	$5{,}5308.10^{3}$	7,5	0,50995
18	$1{,}522.10^{3}$	8,79031	1,29031
19	$6{,}19.10^{2}$	9,68999	0,89968
20	$2{,}517.10^{2}$	10,5899	0,8999
21	$1{,}9.10^{2}$	10,8710	0,2811
22	$1{,}35.10^{2}$	11,2128	0,3418
23	$1{,}1.10^{2}$	11,4176	0,2048
24	$8{,}2.10^{1}$	11,7113	0,2937
25	$6{,}3.10^{1}$	11,9749	0,2636
26	$4{,}5.10^{1}$	12,3114	0,3365
27	$3{,}2.10^{1}$	12,6523	0,3409
28	$2{,}6.10^{1}$	12,8600	0,2077
29	2.10^{1}	13,1223	0,2623
30	$1{,}5.10^{1}$	13,4100	0,2877
31	$1{,}1.10^{1}$	13,7202	0,3102
32	8,0	14,0386	0,3184
33	5,4	14,4317	0,3931
34	3,15	14,9707	0,5390
35	1,84	15,5083	0,5376
36	1,4	15,7816	0,2733
37	$6{,}25.10^{-1}$	16,5881	0,8065
38	$4{,}0.10^{-1}$	17,0344	0,4463
39	$2{,}0.10^{-1}$	17,7275	0,6931
40	0	0	-

Table 3.

Name of element	Resonance groups	Number of ψ functions	
		absorption	fission
TH-232	17 - 29	1	-
U-233		0	0
U-235	27 - 37	8	8
U-238	17 - 33	30	-
PU-239		0	0
PU-240		0	-
PU-241		0	0

APPENDIX A

Calculation of removal rates

Let the limits of macrogroup M be in energy $E_{M-1} > E_M$, in lethargy $u_{M-1} < u_M$ and in microgroup index $(j_{M-1} + 1) \leq j_M$. The contribution of the inelastic scattering is easy to calculate:

$$I_M^R = \sum_{j \in M} \sum_{i > j_M} a_{ij} \Sigma_j^I \phi_j \qquad /86/$$

and

$$I_{M' \to M} = \sum_{j \in M'} \sum_{i \in M} a_{ij} \Sigma_j^I \phi_j \qquad /87/$$

if $M' < M$ else $I_{M' \to M} = 0$.

The elastic contributions are written as a sum of analogous contributions from the various elements:

$$Q_M^R = \sum_k Q_{k,M}^R \qquad /88/$$

and

$$Q_{M' \to M} = \sum_k Q_{M' \to M}^k \qquad /89/$$

Now if for an element

$$u_M - u_{M-1} \geq -\log \alpha_k \qquad /90/$$

or, in other words, the k^{th} element can not scatter across macrogroup M then

$$Q^R_{k,M} = q_{kj_M} \qquad /91a/$$

This is always true for the Fermi-elements:

$$Q^R_{F,M} = q_{F,j_M} \qquad /91b/$$

and for some of the f-elements. For the rest of f-elements $Q^R_{f,M}$ may be written as

$$Q^R_{f,M} = \sum_{j \in M} \Sigma^s_{f,j}\, \phi_j\, w_j \qquad /91c/$$

where w_j is the probability that a neutron scattered in microgroup j gets an energy outside macrogroup M:

$$w_j = \int_{u_{j-1}}^{u_j} \frac{du}{\Delta u_j} \int_{u_M}^{u-\log\alpha_f} du'\, \frac{e^{-(u-u')}}{1-\alpha_f} =$$

$$= \frac{1}{1-\alpha_f} \left[\frac{E_{j_M}}{E_j} \frac{1 - E_j/E_{j-1}}{\Delta u_j} - \alpha_f \right] \qquad /92/$$

The terms $Q^k_{M' \to M}$ on the right hand side of Eq. /89/ are calculated in a similar way. For Fermi-elements

$$Q^F_{M' \to M} = \begin{cases} q_{F j_{M'}} & \text{if} \quad M = M' + 1 \\ 0 & \text{otherwise} \end{cases} \qquad /93a/$$

For f-elements

$$Q^f_{M' \to M} = 0 \qquad \text{if} \qquad u_{M'} - \log\alpha_f \leq u_{M-1} \qquad /93b/$$

i.e. if macrogroups M' and M are too distant for the element, while

$$Q^{f}_{M'\to M} = q_{f j_{M'}} \qquad \text{if} \qquad M = M' + 1 \qquad /93c/$$

and if inequality /90/ holds for both M' and M. In all other cases

$$Q^{f}_{M'\to M} = \sum_{j=j_f}^{j_{M'}} \Sigma^{s}_{fj}\, \phi_j\, w^{M}_{j} \qquad /93d/$$

where w^{M}_{j} is the probability that a neutron scattered in microgroup j gets an energy in macrogroup M and

$$j_f = \max\left(j^*,\ j_{M'-1} + 1\right) \qquad /94a/$$

where j^* satisfies the condition

$$u_{j^*-1} \leq u_{M-1} + \log\alpha_f < u_{j^*} \qquad /94b/$$

Finally, w^{M}_{j} is given similarly to Eq. /92/:

$$w^{M}_{j} = \int_{u^*}^{u_j} \frac{du}{\Delta u_j} \int_{u_{M-1}}^{u^{**}} du'\ \frac{e^{-(u'-u)}}{1-\alpha_f} \qquad /95a/$$

where

$$u^* = \max\left(u_{j-1},\ u_{M-1} + \log\alpha_f\right) \qquad /96a/$$

and

$$u^{**} = \min\left(u_M,\ u - \log\alpha_f\right) \qquad /96b/$$

The integration in Eq. /95a/ can be easily carried out and the result is

$$w_j^M \cdot (1-\alpha_f)\ \Delta u_j = \begin{cases} \left(E_{M-1} - E_M\right)\left(\frac{1}{E_j} - \frac{1}{E^*}\right) & \text{if} \quad u_M + \log\alpha_f < u^* \\ E_{M-1}\left(\frac{\alpha_f}{E_M} - \frac{1}{E^*}\right) - \alpha_f\left(u_M + \log\alpha_f - u^*\right) + \left(E_{M-1} - E_M\right)\left(\frac{1}{E_j} - \frac{\alpha_f}{E_M}\right) & \\ & \text{if} \quad u^* \leq u_M + \log\alpha_f < u_j \\ E_{M-1}\left(\frac{1}{E_j} - \frac{1}{E^*}\right) - \alpha_f\left(u_j - u^*\right) & \text{if} \quad u \leq u_M + \log\alpha_f \end{cases}$$

/95b/

where E^* is the energy corresponding to u^* i.e.

$$E^* = \min\left(E_{j-1}\ ,\ \alpha_f\, E_{M-1}\right) \qquad /96c/$$

Printed in the Central Research Institute
for Physics, Budapest, Hungary
Kiadja a KFKI Könyvtár és Kiadói Osztály
O.v.: Dr. Farkas Istvánné
Szakmai lektor: Kosály György
Nyelvi lektor: Bod László
Példányszám: 187 Munkaszám: 5012
Készült a KFKI házi sokszorositójában
Felelős vezető: Gyenes Imre