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TERMIDOR
AN IBM 7090 FORTRAN CODE TO EVALUATE THE THERMAL NEUTRON SPECTRUM IN AN ORGEL TYPE FUEL ELEMENT

by

G. ROSSI

1962

Joint Nuclear Research Center
Ispra Establishment - Italy

Reactors Physics Department
Applied Physics and Mathematics

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T E R M I D O R

AN IBM 7090 FORTRAN CODE TO EVALUATE THE THERMAL NEUTRON SPECTRUM IN AN ORGEL TYPE FUEL ELEMENT

SUMMARY

The general lines are presented of the simplified model adopted to evaluate the thermal neutron spectrum in an Orgel type fuel element. The flow chart of the code, the input and output data of the subroutines, which contain directly utilisable results, are given.

It is reasonable to admit, at least as a first approximation, that the hardening of the spectrum due to the absorption in the fuel element and the heating effect due to the scattering interaction of the neutrons with the hot coolant, are independent from one another[1].
As a consequence, the two overlapping thermal group approximation, which has been found in good agreement with more fundamental theories in the case of no absorption, can be applied to the description of the pure heating effect in the fuel element.

The energy distributions of the two groups are the Maxwellian ones, respectively at the temperature of the moderator $T_1 = T_m$ and at the temperature

$$T_2 = \frac{\sum_i (\xi \Sigma_s V)_i \, T_i}{\sum_i (\xi \Sigma_s V)_i}$$

obtained by averaging the temperatures of the hot materials contained in the fuel element.
We have therefore

$$\varphi(r, E) = \varphi_1(r) M(E, T_1) + \varphi_2(r) M(E, T_2).$$

The considered regions are separated by the insulating gap and contain 1) moderator and calandria tube, 2) fuel rods, canning sheaths, coolant, graphite fillers, pressure tube (the different materials being homogenized in each region).
The unknowns of the problem are the coefficients $\varphi_1^{(i)}(r)$, $\varphi_2^{(i)}(r)$, which determine in every point r of the region (i) the superposition of the two Maxwellian distributions, by which the spectrum is described.

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(1) In the following, continous reference is made to the paper "A simplified model for the determination of the thermal neutron spectrum in a fuel element" by A. Kind and G. Rossi (to be published in "Energia Nucleare").

These coefficients are solutions of a system of partial differential equations of the two group diffusion type, which are written on the basis of simple balance considerations ; they are linear combinations of modified Bessel functions of the first and second kind. The arbitrary constants are fixed by solving a system of algebric linear equations, which gives the boundary conditions. The matrix of the coefficients of this system and the general expression of the fluxes $\varphi_1^{(i)}(r)$, $\varphi_2^{(i)}(r)$ $(i=1,2)$ are reported in the appendix.

After the fluxes $\varphi_j^{(i)}(r)$ have been tabulated and averaged over the regions 1 and 2, it is possible to calculate effective thermal cross sections for the materials contained in these regions, taking into account the pure heating effect due to the collisions with the coolant nuclei (re-thermalization).(1)

The effective cross section evaluation is carried out through the following procedure (we refer to the point r of the region i, but the results are immediately extended to a whole region by substituting the average values to the values in the point r) :

$$\varphi^{(i)}(r,E) = \varphi_1^{(i)}(r)\, M(E,T_1) + \varphi_2^{(i)}(r)\, M(E,T_2)$$

$$\varphi^{(i)}(r) = \varphi_1^{(i)}(r) + \varphi_2^{(i)}(r)$$

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(1) In the calculation method for ORGEL type lattices, the hardening effect due to the absorption and the epithermal effects are not determined by theoretical methods, but they are taken into account by the results of a "correlation" : for that reason the effective cross sections so determined can be directly introduced in the Orgel lattice calculation (see "Caroline I, une méthode de calcul pour les réseaux eau lourde-organique non irradiés" by G. Casini et al., Euratom internal report ISP - 217 - R).

$$\hat{\varphi}^{(i)}(r) \equiv \int_0^\infty \varphi^{(i)}(r,E)\sqrt{\frac{E_0}{E}}\,dE = \sqrt{\frac{\pi T_0}{4T_1}}\,\varphi_1^{(i)}(r) + \sqrt{\frac{\pi T_0}{4T_2}}\,\varphi_2^{(i)}(r)$$

$$R^{(i)}(r) \equiv \int_0^\infty \sigma(E)\,\varphi^{(i)}(r,E)\,dE$$

$$\hat{\sigma}^{(i)}(r) \equiv \frac{R^{(i)}(r)}{\hat{\varphi}^{(i)}(r)} = \frac{\int_0^\infty \sigma(E)\,\varphi^{(i)}(r,E)\,dE}{\sqrt{\frac{\pi T_0}{4T_1}}\,\varphi_1^{(i)}(r) + \sqrt{\frac{\pi T_0}{4T_2}}\,\varphi_2^{(i)}(r)}\,.$$

In the case of "1/v" absorbers, $\sigma(E) = \sigma_0\sqrt{\frac{E_0}{E}}$, we get $\hat{\sigma} = \sigma_0$; in a general way, if the Westcott's g(T) curve for the considered process is known, we get :

$$(1) \qquad \hat{\sigma}^{(i)}(r) = \frac{g(T_1)\sqrt{\frac{\pi T_0}{4T_1}}\,\varphi_1^{(i)}(r) + g(T_2)\sqrt{\frac{\pi T_0}{4T_2}}\,\varphi_2^{(i)}(r)}{\sqrt{\frac{\pi T_0}{4T_1}}\,\varphi_1^{(i)}(r) + \sqrt{\frac{\pi T_0}{4T_2}}\,\varphi_2^{(i)}(r)}\,\sigma_0$$

$$\equiv g(T_1, T_2, r)\,\sigma_0$$

$$(2) \qquad \bar{\sigma}^{(i)}(r) = \frac{R^{(i)}(r)}{\hat{\varphi}^{(i)}(r)} \cdot \frac{\hat{\varphi}^{(i)}(r)}{\varphi^{(i)}(r)} = \hat{\sigma}^{(i)}(r)\,\frac{\hat{\varphi}^{(i)}(r)}{\varphi^{(i)}(r)}$$

$$= \hat{\sigma}^{(i)}(r)\,\frac{\sqrt{\frac{\pi T_0}{4T_1}}\,\varphi_1^{(i)}(r) + \sqrt{\frac{\pi T_0}{4T_2}}\,\varphi_2^{(i)}(r)}{\varphi_1^{(i)}(r) + \varphi_2^{(i)}(r)}\,.$$

To compare theoretical with experimental results, it can be useful to determine a neutron effective temperature in a point $\underline{r}$ of the cell, with reference for instance to the fission reaction rate ratio of Pu_{239} and U_{235}. This effective temperature is calculated by solving the equation :

$$(3) \qquad \frac{g_{9f}(T_1, T_2, r)}{g_{5f}(T_1, T_2, r)} = \frac{g_{9f}(T)}{g_{5f}(T)} .$$

The "homogeneous" hardening effect is taken into account by shifting the "temperature" of the Maxwellian, which represents the spectrum entering the fuel element, by a quantity ΔT obtained by means of semi-empirical formulae (Brown and St.John ; Coveyou, Bate and Osborne), provided the absorbers are diluted on the whole cell.

The "heterogeneous" hardening effect on a so modified incoming Maxwellian is determined in the framework of a multigroup diffusion model (selective diffusion). On the basis of the hypothesis, that the hardening process and the rethermalization are independent from one another, the neutron transfer between the groups, due to the interaction with the moderating materials contained in the fuel element, is neglected.
By averaging on the fuel element, we obtain a spectrum F(E), which takes into account the pure hardening effect and depends on the "temperature" of incoming Maxwellian as well as on the coolant density :

$$(4) \qquad F(E) = \frac{b^2 - a^2}{a\, I(a)} \cdot \frac{I_1[\varkappa_f(E)\, a]}{\varkappa_f(E)\, a} \cdot \frac{M(E, T'_m)}{I_0[\varkappa_f(E) a] + 2 D_f(E) \varkappa_f(E) I_1[\varkappa_f(E) a]} ,$$

where

a = fuel element radius

b = equivalent cell radius

$$I(a) = \int_0^\infty dE\, M(E,T'_m) \frac{D_f(E)\,\varkappa_f(E)\,I_1[\varkappa_f(E)a]}{I_0[\varkappa_f(E)a] + 2D_f(E)\varkappa_f(E)I_1[\varkappa_f(E)a]},$$

$$\varkappa_f^2(E) = \frac{\Sigma_{af}(E)}{D_f(E)}$$

(the suffix "f" denotes the fuel element),

T'_m = temperature of the "incoming" Maxwellian.

A thermal neutron spectrum in the fuel element, which takes into account the hardening process and the rethermalization at the same time, can be given in two limit cases :

a) when the rethermalization mean free path goes to zero, we can admit that only the neutrons which did not interact with the coolant nuclei are affected by the hardening process. This hypothesis brings to the following description of the spectrum in the fuel element :

$$(5) \qquad \Phi_1(E) = \langle \varphi_1^{(2)}(r) \rangle F(E) + \langle \varphi_2^{(2)}(r) \rangle M(E,T_2) ;$$

b) when the rethermalization mean free path becomes very large, the independence hypothesis is well verified, and we have a pure superposition of the effects ; the spectrum is given by (4), provided we substitute the incoming Maxwellian with the rethermalized spectrum :

$$(6) \quad \Phi_2(E) = \frac{b^2 - a^2}{a\,I^*(a)} \cdot \frac{1}{\varkappa_f(E)a} \cdot I_1[\varkappa_f(E)a] \cdot \frac{\langle \varphi_1^{(2)}(r) \rangle M(E,T_1) + \langle \varphi_2^{(2)}(r) \rangle M(E,T_2)}{I_0[\varkappa_f(E)a] + 2D_f(E)\varkappa_f(E)I_1[\varkappa_f(E)a]},$$

where

$$I^*(a) = \int_0^\infty dE \left[\langle \varphi_1^{(2)}(r) \rangle M(E,T_1) + \langle \varphi_2^{(2)}(r) \rangle M(E,T_2) \right] \frac{D_f(E)\varkappa_f(E)I_1[\varkappa_f(E)a]}{I_0[\varkappa_f(E)a] + 2D_f(E)\varkappa_f(E)I_1[\varkappa_f(E)a]}.$$

For each of these spectrum expressions, opportunely normalized, an effective neutron temperature in the fuel element by means of a relationship such as (3) can be calculated, by introducing on the left hand-side the reaction rates evaluated through numerical integration. In this manner a neutron temperature range, where the experimental value should be found, is obtained.

To interpolate between these limits, the following formula is proposed :

$$(7) \qquad T_n = T_{n1} + \left[1 - \exp\left(-\frac{\lambda_{reth}}{\lambda_a}\right)\right](T_{n2} - T_{n1}).$$

An IBM 7090 FORTRAN code named TERMIDOR (TERMalizzazione Deuterio ORganico) was written[1], which allows, for a generical heavy water moderated organic cooled lattice, the calculation of the following quantities :

"fluxes" $\varphi_1^{(i)}(r)$, $\varphi_2^{(i)}(r)$ $\qquad (i=1,2)$

- average values of the "fluxes" in the fuel element
- thermal effective cross sections for the materials in the fuel element to be introduced in Orgel lattice calculations (i.e. which take into account the pure rethermalization effect)
- neutron effective temperature in the fuel element, with reference to the fission reaction rate ratio Pu_{239}/U_{235}, which takes into account the pure rethermalization effect (from which the coolant temperature coefficient $\Delta T_n / \Delta T_{org}$ can be inferred).
- "total" fuel element spectrum $\phi_1(E)$, $\phi_2(E)$ in the two above mentioned limit cases a), b)

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(1) The programming work was mainly done by Miss C. Vinche.

- neutron effective temperatures corresponding to these limit cases.

In the appendix are given

- the "flow chart" of the code
- the input data with their "format"
- the output data of the two last subroutines.

APPENDIX

1) GENERAL SOLUTIONS OF THE TWO THERMAL GROUP, TWO CYLINDRICAL REGION DIFFUSION EQUATIONS (*/.)
2) MATRIX OF THE COEFFICIENTS OF THE BOUNDARY CONDITION SYSTEM (*/.)
3) FLOW CHART OF THE TERMIDOR CODE (*/.)

4) INPUT DATA OF THE TERMIDOR CODE.

   a) FORMAT (I4)

      J (= 1 for U metal ; = 2 for UO_2 ; = 3 for UC)

      JCAN (= 1 for Al sheaths (SAP) ; = 2 for Zr sheaths (Zircaloy))

      JTU (Id. for pressure tube)

      JCAL (Id. for calandria tube)

   b) FORMAT (F8.4)

      W enrichment (Co)

      DUØ2 UO_2 density

      DUC UC density

      T1 D_2O temperature (°K)

Z	weight fraction of Mo in the Uranium metal alloy
S	radius of the uncanned rodlet
AB	radius of the homogenized rod
A	inner radius of pressure tube
A3	outer radius of pressure tube
VØ1	coolant volume in the homogenized rod
VGR1	graphite volume in the homogenized rod
VØ2	coolant volume in the outer shell
VGR2	graphite volume in the outer shell
B	radius of the equivalent cell
R2	radius of the hot region (= A3)
R1	radius of the cold region (= B)
VB	volume of the homogenized rod
VC	volume of the fuel
VG	total sheaths volume
VT	volume of the pressure tube
VV	volume of the insulating gap
A4	outer radius of calandria tube
VCA	volume of calandria tube
TAU	burn up value

c) FORMAT (F8.4)

T2	coolant temperature (°K)
TN1	temperature of the cold Maxwellian (°K)
TN2	temperature of the hot Maxwellian (°K)
XKTM	temperature of the Maxwellian incoming in the fuel element (ev)

N.B. Many series of values of the last four data can be given at the same time.

5) OUTPUT DATA OF THE TERMIDOR CODE.

The results of the two last subroutines are only reported : the results of the preceeding ones are intermediate.

SUBROUTINE 8 FORMAT (5E20.5) (= 5 results for each line)

F2M(1), F2M(2) average values of the $\varphi_1(r)$, $\varphi_2(r)$ in the fuel element

XVT95F neutron effective temperature in the fuel element referred to the fission ratio Pu_{239}/U_{235}

ALAM $= \dfrac{\varphi_1^{(2)}(r_2)\sqrt{\frac{nT_o}{4T_{n1}}} + \varphi_2^{(2)}(r_2)\sqrt{\frac{nT_o}{4T_{n2}}}}{\varphi_1^{(2)}(r_2) + \varphi_2^{(2)}(r_2)} = \dfrac{\overline{\sigma}(r_2)}{\sigma_o}$ for "$\frac{1}{v}$" absorber

ALAM2 = id. with $\langle\varphi_i^{(2)}(r)\rangle$ instead of $\varphi_i^{(2)}(r_2)$

SCA9 fuel effective cross section

FORMAT (4E20.5)

G5AM $= g_{5a}^{(2)}(T_{n1}, T_{n2})$

G5AMV = G5AM * ALAM2

G5FM $= g_{5f}^{(2)}(T_{n1}, T_{n2})$

G5FMV = G5FM * ALAM2

G9AM , G9AMV , G9FM , G9FMV

GOAM , GOAMV , G1AM , G1AMV

SUBROUTINE HETHARD. FORMAT (2E20.5)

XVT1 , XVT2 neutron effective temperature in the limit cases.

Tabulation of the fuel element spectra in the limit cases FAVN1 , FAV2 (arbitrary units) as a function of the energy E(ev).

app. 1

$$\varphi_1^{(2)}(r) = A_1^{(2)}\, I_0(\eta_1^{(2)} r) \qquad (0 \leqslant r \leqslant r_2)$$

$$\varphi_2^{(2)}(r) = A_2^{(2)}\, I_0(\epsilon_2^{(2)} r) + \frac{\sum_{1\to 2}^{(2)} D_2}{\left[\epsilon_2^{(2)}\right]^2 - \left[\eta_1^{(2)}\right]^2} A_1^{(2)}\, I_0(\eta_1^{(2)} r) + \frac{q_2}{\sum_{a_2}^{(2)}} \qquad (0 \leqslant r \leqslant r_2)$$

$$\varphi_2^{(1)}(r) = A_2^{(1)}\, I_0(\eta_2^{(1)} r) + B_2^{(1)}\, K_0(\eta_2^{(1)} r) \qquad (r_2 \leqslant r \leqslant r_1)$$

$$\varphi_1^{(1)}(r) = A_1^{(1)}\, I_0(\epsilon_1^{(1)} r) + B_1^{(1)}\, K_0(\epsilon_1^{(1)} r) + \frac{\sum_{2\to 1}^{(1)} D_1}{\left[\epsilon_1^{(1)}\right]^2 - \left[\eta_2^{(1)}\right]^2} \varphi_2^{(1)}(r) + \frac{q_1}{\sum_{a_1}^{(1)}} \qquad (r_2 \leqslant r \leqslant r_1)$$

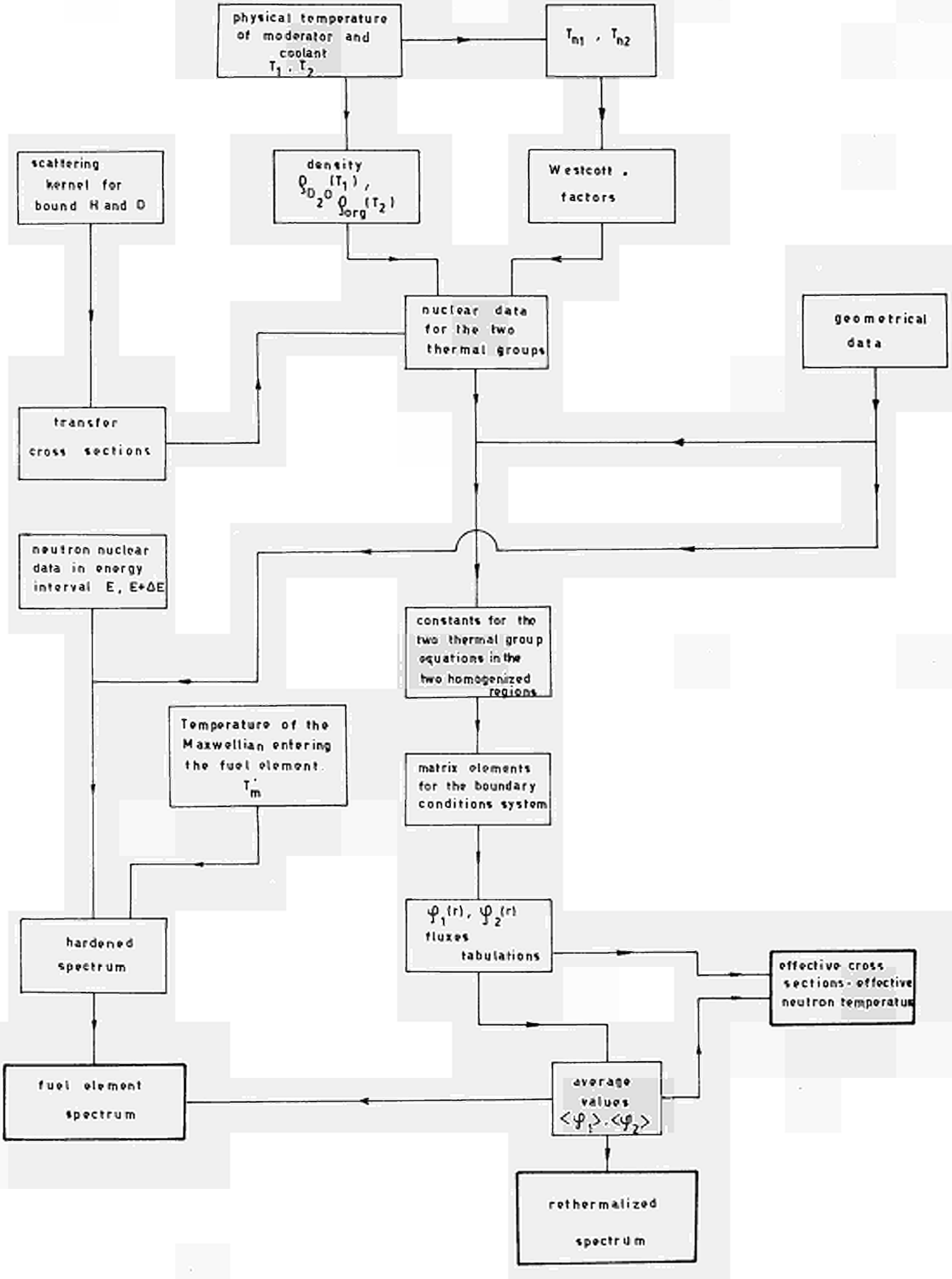
$$\left[\eta_1^{(2)}\right]^2 = \frac{\sum_{a_1}^{(2)} + \sum_{1\to 2}}{D_1^{(2)}} \qquad \left[\epsilon_1^{(1)}\right]^2 = \frac{\sum_{a_1}^{(1)}}{D_1^{(1)}}$$

$$\left[\eta_2^{(1)}\right]^2 = \frac{\sum_{a_2}^{(1)} + \sum_{2\to 1}}{D_2^{(1)}} \qquad \left[\epsilon_2^{(2)}\right]^2 = \frac{\sum_{a_2}^{(2)}}{D_2^{(2)}}$$

$$A_1^{(2)} = 1, \qquad q_2 = q_1 \times \frac{(\xi \Sigma_s V)_r}{(\xi \Sigma_s V)_m}$$

$A_2^{(2)}, A_2^{(1)}, A_1^{(1)}, B_2^{(1)}, B_1^{(1)}, q_1$ are the solutions of a six algebric equations system, which represent the boundary conditions.

$A_1^{(1)}$	$A_2^{(1)}$	$A_2^{(2)}$	$B_1^{(1)}$	$B_2^{(1)}$	q_1	known term
$I_o(\varepsilon_1^{(1)} r_2)$	$\frac{\sum_{2\to1} D_1^{(1)}}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2} I_o(\eta_2^{(1)} r_2)$		$K_o(\varepsilon_1^{(1)} r_2)$	$\frac{\sum_{2\to1} D_1^{(1)}}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2} K_o(\eta_2^{(1)} r_2)$	$\frac{1}{\sum_{a_1}^{(1)}}$	$I_o(\eta_1^{(2)} r_2)$
	$I_o(\eta_2^{(1)} r_2)$	$-I_o(\varepsilon_2^{(2)} r_2)$		$K_o(\eta_2^{(1)} r_2)$	$-\frac{(\sum\sum_s V)_r / (\sum\sum_s V)_m}{\sum_{a_2}^{(2)}}$	$\frac{\sum_{1\to2} D_2^{(2)}}{[\varepsilon_2^{(2)}]^2 - [\eta_1^{(2)}]^2} I_o(\eta_1^{(2)} r_2)$
$D_1^{(1)} \varepsilon_1^{(1)} I_1(\varepsilon_1^{(1)} r_2)$	$\frac{\sum_{2\to1} \eta_2^{(1)} I_1(\eta_2^{(1)} r_2)}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2}$		$-D_1^{(1)} \varepsilon_1^{(1)} K_1(\varepsilon_1^{(1)} r_2)$	$\frac{\sum_{2\to1} \eta_2^{(1)} K_1(\eta_2^{(1)} r_2)}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2}$		$D_1^{(2)} \eta_1^{(2)} I_1(\eta_1^{(2)} r_2)$
	$D_2^{(1)} \eta_2^{(1)} I(\eta_2^{(1)} r_2)$	$-D_2^{(2)} \varepsilon_2^{(2)} I_1(\varepsilon_2^{(2)} r_2)$		$-D_2^{(1)} \eta_2^{(1)} K_1(\eta_2^{(1)} r_2)$		$\frac{\sum_{1\to2} \eta_1^{(2)} I_1(\eta_1^{(2)} r_2)}{[\varepsilon_2^{(2)}]^2 - [\eta_1^{(2)}]^2}$
$\varepsilon_1^{(1)} I_1(\varepsilon_1^{(1)} r_1)$	$\frac{\sum_{2\to1} D_1^{(1)} \eta_2^{(1)} I_1(\eta_2^{(1)} r_1)}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2}$		$-\varepsilon_1^{(1)} K_1(\varepsilon_1^{(1)} r_1)$	$\frac{-\sum_{2\to1} D_1^{(1)} \eta_2^{(1)} K_1(\eta_2^{(1)} r_1)}{[\varepsilon_1^{(1)}]^2 - [\eta_2^{(1)}]^2}$		
	$\eta_2^{(1)} I_1(\eta_2^{(1)} r_1)$			$\eta_2^{(1)} K_1(\eta_2^{(1)} r_1)$		


physical temperature of moderator and coolant T_1 . T_2
T_{n1} , T_{n2}
scattering kernel for bound H and D
density $\varrho_{D_2O}(T_1)$, $\varrho_{org}(T_2)$
Westcott . factors
nuclear data for the two thermal groups
geometrical data
transfer cross sections
neutron nuclear data in energy interval E, E+ΔE
constants for the two thermal group equations in the two homogenized regions
Temperature of the Maxwellian entering the fuel element T_m
matrix elements for the boundary conditions system
$\varphi_1(r)$, $\varphi_2(r)$ fluxes tabulations
effective cross sections - effective neutron temperatur
hardened spectrum
fuel element spectrum
average values $\langle\varphi_1\rangle$. $\langle\varphi_2\rangle$
rethermalized spectrum

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