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A SIMPLIFIED MODEL FOR THE DETERMINATION OF THE THERMAL NEUTRON SPECTRUM IN A FUEL ELEMENT

by

A. KIND et G. ROSSI

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Joint Nuclear Research Centre
Ispra Establishment (Italy)

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1. INTRODUCTION

A typical phenomenon occurring in fuel elements containing moderating materials, such as for instance the coolant, is the neutron rethermalization. The neutrons which have been slowed down in the main moderator to an energy distribution determined essentially by the temperature of this medium, when entering the fuel element undergo collisions with the light nuclei of the moderating material at high temperature. By this interaction they are partly transferred to a new energy distribution characterized by a higher « temperature ». At the same time, due to the selective absorption in the fuel, their energy spectrum is progressively hardened through the fuel element.

A complete and rigorous description of the thermal neutron spectrum in a fuel element can be in principle obtained by means of elaborated methods such as, for instance, the Monte Carlo method or « numerical » resolutions of the space-energy Boltzmann equation. This, under the condition that the scattering kernel describing the interaction of the neutrons with the nuclei bounded in the coolant molecules is known.

This generally leads to heavy numerical calculations with the necessity of using big electronic computers. It seems therefore useful, in view of design analyses, to dispose of a simple method which, although reproducing correctly the essential physical situation, does not imply the use of heavy numerical calculations.

A possibility in this line seems to be given by the assumption that the two effects, the hardening due to the selective absorption, and the rethermalization due to interaction with the coolant nuclei, are independent from one another. In this case, these effects can be treated separately, each by the use of simple methods.

A simple method to treat the rethermalization is the two overlapping thermal group approximation [1] used by disregarding every distortion of the spectrum due to the absorption, i.e. by choosing for the energy distributions related to the two thermal groups the maxwellian ones at the physical temperatures of the moderator and of the coolant.

With regard to the hardening, the simplification may consist in disregarding, in the framework of a multigroup diffusion model [2], the transfer of neutrons

from one energy group to the other due to the interaction with the moderating materials.
The independence hypothesis regarding the two phenomena taking place in the fuel element can in a general way be justified only by the consideration that the interference between two effects which can be treated as perturbations, may be considered as small. It is not easy to fix on this basis the limits of applicability of this approximation. One can in principle say that this approximation is all the more justified as the rethermalization effect in the fuel element is smaller. On the other hand, it must be pointed out that, in the framework of the gas model, the quantity describing the transfer of neutrons from the « cold » to the « hot » group (rethermalization cross section) comes out to be in good approximation independent from the shape of the « incoming » spectrum. Therefore, the influence of the hardening on the rethermalization effect can be considered as small, also by strong absorption.
In the following, the proposed method is described together with the results which have been obtained by its application to a D_2O moderated and cooled cell for which spectrum measurements have been performed at Chalk River.

2. THE TWO THERMAL GROUP APPROXIMATION

In the original Selengut formulation of the method[1] the thermal neutron flux in a cell with a temperature discontinuity, is written:

$$\phi(r, E) = \chi_1(E)\,\phi_1(r) + \chi_2(E)\,\phi_2(r) \qquad (2.1)$$

where $\chi_i(E)$ represents the « equilibrium » energy distribution of the neutrons in the medium (i); $\phi_1(r)$, $\phi_2(r)$ are solutions of equations the formulation of which is based on elementary balance considerations (1 refers to the main moderator, 2 to the region containing the moderating nuclei at higher temperature).
In region (1), which contains the main moderator and the cold structural materials, the equations, in the diffusion approximation, are the following:

$$\begin{aligned} -D_1^{(1)}\nabla^2\phi_1^{(1)} + \Sigma_{a1}^{(1)}\phi_1^{(1)} &= \sum_{2\to1}\phi_2^{(1)} + q_1 \\ -D_2^{(1)}\nabla^2\phi_2^{(1)} + \Sigma_{a2}^{(1)}\phi_2^{(1)} + \sum_{2\to1}\phi_2^{(1)} &= 0 \end{aligned} \qquad (2.2)$$

In region (2), which contains fuel, coolant and hot structural materials, they are:

$$\begin{aligned} -D_1^{(2)}\nabla^2\phi_1^{(2)} + \Sigma_{a1}^{(2)}\phi_1^{(2)} + \sum_{1\to2}\phi_1^{(2)} &= 0 \\ -D_2^{(2)}\nabla^2\phi_2^{(2)} + \Sigma_{a2}^{(2)}\phi_2^{(2)} &= \sum_{1\to2}\phi_1^{(2)} + q_2 \end{aligned} \qquad (2.3)$$

The upper label (i) indicates the region, the lower one j the energy distribution over which the quantity is averaged; q_i is the slowing down source (supposed to be constant in each region) and $\sum_{i\to j}$ the transfer cross-section from the $\chi_i(E)$ to the $\chi_j(E)$ distribution.
The calculations are particularly simple and the method is suitable for current design evaluations, provided the distributions $\chi_i(E)$ are supposed to be maxwellian:

$$\chi_1(E) \equiv M(E, T_1) \qquad \chi_2(E) \equiv M(E, T_2) \qquad (2.4)$$

By fixing the temperatures T_1 and T_2 of the maxwellian distributions as functions of the physical temperatures T_m, T_c of moderator and coolant, the fluxes $\phi_i(r)$ can be determined and, according to the Westcott formalism, the reaction rates for thermal neutrons in the fuel element get the form:

$$\begin{aligned} < R(T_m, T_c, r) >_f = [g(T_1) < \hat{\phi}_1(r) >_f + \\ + g(T_2) < \hat{\phi}_2(r) >_f]\,\Sigma_0 \end{aligned} \qquad (2.5)$$

(where the symbol $< >_f$ indicates the space average over the fuel element and Σ_0 is the macroscopic cross-section for a suitable fixed test event). A neutron equivalent « temperature » averaged over the fuel rod $< T_n >_f$ can be defined by the relation:

$$< R(T_m, T_c, r) >_f = g(T)\,\Sigma_0 < \hat{\phi}(r) >_f \qquad (2.6)$$

where $\hat{\phi} = \hat{\phi}_1 + \hat{\phi}_2$.

In the case of no absorption, the correct solution for $\phi(r, E)$ would be obtained by putting $T_1 = T_m$ and $T_2 = T_c$ and by solving the equations (2.2) and (2.3): the results have been found to be in good agreement with those of more sophisticated methods [3]. On the contrary, in a fuel element, a

correct spectrum determination by means of a two overlapping thermal group approximation would be possible, only recurring to a rather complex variational procedure [4].

However, in the framework of our model, the spectral distortions due to the absorptions are introduced separately and, in the above-described formalism, the « temperatures » of the maxwellians have to be taken equal to the physical temperatures of the moderating materials.

Following this line, the quantity $\frac{\Delta T_n}{\Delta T_c}$ (variation of the neutron temperature in the fuel element following a unit variation of the coolant temperature), which is of primary interest for the knowledge of the coolant temperature coefficient, can be calculated — at least in first approximation — in a simple and suggestive manner.

The materials of the cell have been homogenized to get a hot and a cold region. The constants of equations (2.2) and (2.3) are obtained by averaging over the neutron energy distribution and over the volumes and fluxes, following the usual one group flux fine structure calculation. The solutions of equations (2.2) and (2.3) are linear combinations of modified Bessel functions of the first and second kind; the arbitrary constants are determined by solving a linear algebric equation system, which describes the boundary conditions.

From the physical point of view, the fundamental problem is the determination of the probability that a neutron belonging to one of the two groups is transferred to the other, i.e. the determination of the rethermalization cross-sections. These are defined as it is usually done in the multigroup models, by means of the average energy change $< \Delta E >_{ij}$ of a neutron belonging to the $M(E, T_j)$ distribution, following a collision in a medium at the temperature T_i. In terms of the scattering kernel $\sigma_s(E \to E', T)$ for the neutrons at the energy E colliding in a medium at the temperature T, it is given by:

$$< \Delta E >_{ij} = \int\int (E' - E)\, \sigma_s(E \to E', T_i) \cdot M(E, T_j)\, dE'\, dE \qquad (2.7)$$

This quantity is dependent on the model adopted to describe the neutron scattering by the coolant nuclei. Although very refined evaluations are possible, we have adopted the free gas model, with an effective mass value to take into account the chemical bound.

By introducing in equation (2.7) the scattering kernel of the heavy gas model, the very simple result is obtained:

$$\sum_{j \to i} = \frac{2}{A}\, \Sigma_s \qquad (2.8)$$

It has been shown [5] that a generalization of (2.8) to scattering nuclei of any mass number is given by:

$$\sum_{j \to i} = \frac{2A}{(A+1)^2}\, \lambda_1\, \Sigma_s \qquad (2.8')$$

where λ_1 is the first eigenvalue $\neq 0$ of the free gas scattering operator for a nucleus of mass A (for $A \geq 3$ it is practically $\lambda_1 = 1$) and Σ_s is the « free atom » cross section.

As regards the effective mass to be attributed to the bound proton and deuteron, some valuable indications can be found in the literature: as regards the proton, we believe that a consistent procedure is given by the systematic adoption of the phenomenological model of Drozdov et al. [6], while for the deuteron bound in D_2O molecule, the model proposed by Brown and St-John [7] can be regarded as sufficiently accurate.

The rethermalizing effect of the hot structural materials and of the nuclei possibly bound to the uranium in the fuel cannot be neglected: this has been recently pointed out by the Canadian experiments.

By considering the hot materials in the fuel element as a homogeneous mixture of heavy free nuclei, it is possible to introduce in the formalism a temperature T_2 defined as follows:

$$T_2 = \frac{(\xi \Sigma_s V)_c T_c + (\xi \Sigma_s V)_g T_g + (\xi \Sigma_s V)_f T_f}{(\xi \Sigma_s V)_c + (\xi \Sigma_s V)_g + (\xi \Sigma_s V)_f} \qquad (2.9)$$

where T_c, T_g, T_f are the physical temperatures of coolant, canning and fuel respectively.

3. THE SPECTRUM HARDENING IN THE FUEL ELEMENT

In order to treat, according to our model, the hardening of the neutron spectrum through the fuel element, the effects of capture and scattering on this spectrum have to be determined by excluding every energy transfer.

Among various possibilities, the way we chose was that of a multigroup diffusion calculation by which every transfer term between different groups is taken equal to zero.

In the assumption that the sources are space independent in the moderator as well as in the fuel element, the equations which describe the space distribution of the thermal neutrons belonging to the energy interval $(E, E + \Delta E)$ are:

$$- D_m(E) \nabla^2 \phi_m(r, E) + \Sigma_{am}(E) \phi_m(r, E) = Q_m(E) \quad (3.1)$$

$$- D_f(E) \nabla^2 \phi_f(r, E) + \Sigma_{af}(E) \phi_f(r, E) = Q_f(E) \quad (3.2)$$

With regard to the sources themselves, we make the two further assumptions: first, their intensities are proportional to the quantities $\xi \Sigma_s V$. Due to the fact that in the cases in which we are interested the ratio $\frac{(\xi \Sigma_s V)_o}{(\xi \Sigma_s V)_m}$ is much smaller than unity, we neglect at this point the source in the fuel element. Secondly, we assume that the source in the moderator is a maxwellian at the moderator temperature:

$$Q_m(E) = Q_{mo} M(E, T_m) \quad (3.3)$$

From equation (3.2) one gets:

$$\phi_f(r, E) = A(E) I_o[\varkappa_f(E) r] \quad \left(\varkappa^2_f(E) = \frac{\Sigma_{af}(E)}{D_f(E)}\right) \quad (3.4)$$

We put furthermore $D_m(E) = \text{const}(E)$ and $\Sigma_{am}(E) = 0$, so that the energy distribution of the neutrons in the moderator comes out to be at any point a maxwellian at the moderator temperature:

$$\phi_m(r, E) = M(E, T_m) \phi_m(r) \quad (3.5)$$

and the solution of the problem is given by the determination of $A(E)$ and $\phi_m(r)$.

The boundary conditions between moderator and fuel element have to be fixed. The most adequate scheme to do this seems to be the one proposed by E. U. Vaughan [2] which consists in the assumption that, while the continuity for the incoming current is requested for every energy group, for the outgoing current only an integral continuity condition over the whole energy range is imposed.

The boundary conditions are then the following:

$$\frac{1}{4} A(E) I_o[\varkappa_f(E) a] + \frac{1}{2} D_f(E) A(E) \left\{ \frac{\partial}{\partial r} I_o[\varkappa_f(E) r] \right\}_a = \frac{1}{4} M(E, T_m) \phi_m(a) + D_m M(E, T_m) \left[\frac{\mathrm{d}}{\mathrm{d}r} \phi_m(r)\right]_a \quad (3.6)$$

$$\int \mathrm{d}E \left\{ \frac{1}{4} A(E) I_o[\varkappa_f(E) a] - \frac{1}{2} D_f(E) A(E) \left[\frac{\partial}{\partial r} I_o(\varkappa_f(E) r)\right]_a \right\} = \frac{1}{4} \phi_m(a) - \frac{1}{2} D_m \left[\frac{\mathrm{d}}{\mathrm{d}r} \phi_m(r)\right]_a \quad (3.7)$$

$$\left[\frac{\mathrm{d}\phi_m(r)}{\mathrm{d}r}\right]_b = 0 \quad (3.8)$$

(a = fuel element radius; b = radius of the equivalent cell).

From these conditions, $A(E)$ and $\phi_m(r)$ are determined for $Q_{mo} = 1$.

One gets:

$$A(E) = \frac{(b^2 - a^2) \frac{1}{2 a I(a)} M(E, T_m)}{I_o[\varkappa_f(E) a] + 2 D_f(E) \varkappa_f(E) I_1[\varkappa_f(E) a]} \quad (3.9)$$

where the quantity $I(a)$ is defined as:

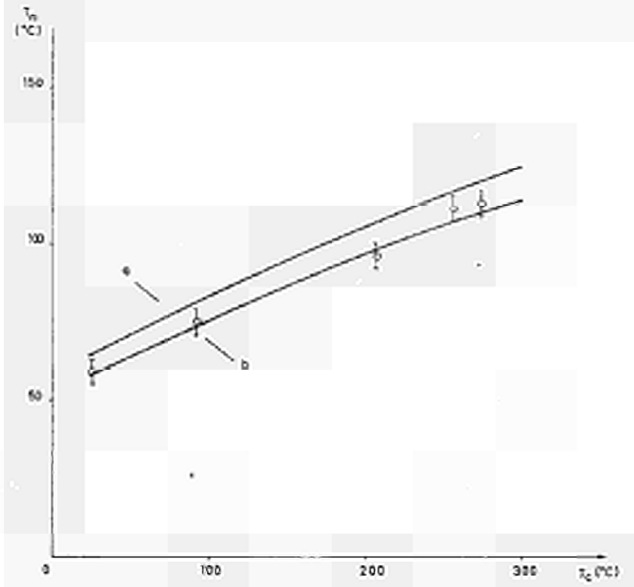

Fig. 1 - Neutron effective temperature in a CANDU type fuel element ($\lambda_{reth} \sim 1.4\ \lambda_a$). a) from formula (4.1); b) from formula (4.2).

$$I(a) = \int_0^\infty dE\, M(E, T_m) \cdot \frac{D_f(E)\, \varkappa_f(E)\, I_1[\varkappa_f(E)\, a]}{I_0[\varkappa_f(E)\, a] + 2\, D_f(E)\, \varkappa_f(E)\, I_1[\varkappa_f(E)\, a]} \quad (3.10)$$

From (3.9) it follows:

$$\dot{\varphi}_f(r, E) = \frac{(b^2 - a^2)\, \dfrac{1}{2\, a\, I(a)}\, M(E, T_m)}{I_0[\varkappa_f(E)\, a] + 2\, D_f(E)\, \varkappa_f(E)\, I_1[\varkappa_f(E)\, a]} \cdot I_0[\varkappa_f(E)\, r] \quad (3.11)$$

and averaging over the fuel element:

$$F(E) = \frac{(b^2 - a^2)\, \dfrac{1}{2\, a\, I(a)}\, M(E, T_m)}{I_0[\varkappa_f(E)\, a] + 2\, D_f(E)\, \varkappa_f(E)\, I_1[\varkappa_f(E)\, a]} \cdot \frac{2}{\varkappa_f(E)\, a} \cdot I_1[\varkappa_f(E)\, a] \quad (3.12)$$

From (3.12) the reaction rate ratio for different detectors averaged over the fuel element can be evaluated and, through a relation similar to (2.6), an effective neutron temperature can be defined.
Finally, to the « heterogenous » hardening due to the selective absorption through the fuel element, the « homogeneous » effect has to be added, which derives from the fact that the neutrons absorbed in the cell come from a non-equilibrium source. This effect can be evaluated by means of expressions like the one of Brown and St. John, once the average absorption cross-section over the cell at $E = K\, T_m$ has been determined.

4. EVALUATION OF THE NEUTRON SPECTRUM IN A FUEL ELEMENT

Once fixed the geometrical and physical characteristics of the cell and the test event by which the neutron effective temperature in the fuel element has to be defined (for instance, the fission reaction rate ratio Pu^{239}/U^{235}), the above-described method allows the determination of the following quantities:

a) $\alpha = \dfrac{\Delta < T_n >_f}{\Delta T_2}$, variation of the mean neutron temperature in the fuel element following a unit variation of the mean temperature in its moderating components (see 2.9);

b) $\Delta T_n = < T_n\ (T_r = T_m) >_f - T_m$, difference between the mean neutron temperature in the fuel element and the main moderator temperature, calculated for $T_r = T_m$ and no neutron energy change in the fuel element.

By means of these two quantities, a full description of the thermal neutron spectrum in the fuel element can be given in first approximation as follows:

$$< T_n >_f = T'_m + \Delta T_n + \alpha\, (T_2 - T'_m) \quad (4.1)$$

where $T'_m - T_m$ represents the « homogeneous » hardening in the cell.
By this expression, every interference between the rethermalization effect and the hardening due to the selective absorption in the fuel is neglected. This corresponds strictly to the lines of our simplified model. Nevertheless, if some attempt has to be made to give a more realistic picture of the processes occurring in the fuel element, it can be done as follows: formula (4.1) describes correctly the limit case by which the rethermalization mean free

path λ_{reth} is big as compared to the mean free path λ_a related to the capture. In this case, the hardening process is unaffected by the scattering collisions with the coolant (see § 1). In the opposite limit case $\lambda_{reth} \ll \lambda_a$, a correct description of the spectrum seems to be possible by assuming that only the neutrons which did not interact with the coolant nuclei are hardened. This brings to the following description of the spectrum in the fuel element:

$$< \phi (r, E) >_f = \frac{< \phi_1 (r) >_f F (E) + < \phi_2 (r) >_f M (E, T_2)}{< \phi_1 (r) >_f + < \phi_2 (r) >_f} \quad (4.2)$$

$F (E)$ is given by the normalized expression (3.12) and the space dependent factors $\phi_1 (r)$ and $\phi_2 (r)$ are the same as the ones obtained by the calculation of the pure rethermalization effect as described in § 2.

It must be pointed out that in the limit case given by (4.2) a full description of the spectrum distortion in the fuel element is possible without the introduction of any effective temperature as it is done by (4.1). A similar possibility is given in the limit case (4.1) too, if assuming for the mean spectrum in the fuel element the expression (3.12) in which the entering maxwellian distribution $M (E, T_m)$ has been substituted by the rethermalized spectrum:

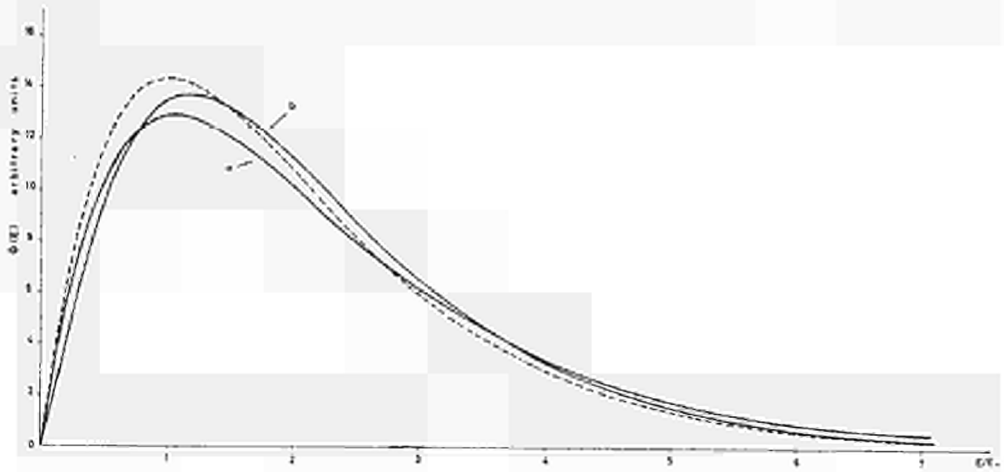

Fig. 2 - ——— Maxwellian at 23 °C. a) Rethermalized spectrum for T_2 = 250 °C; b) Hardened spectrum (from formula (3.12)).

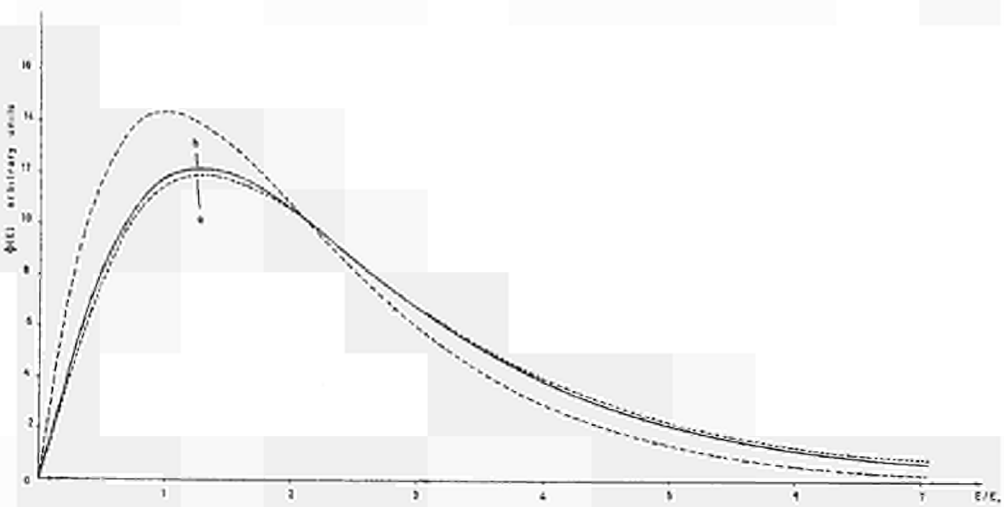

Fig. 3 - ——— Maxwellian at 23 °C. a) Rethermalized and hardened spectrum for T_2 = 250 °C (from formulae (3.12) and (4.3)); b) Idem (from formula (4.2)).

$$F_{\text{reth}}(E) =$$

$$= \frac{<\phi_1(r)>_f M(E,T_m) + <\phi_2(r)>_f M(E,T_2)}{<\phi_1(r)>_f + <\phi_2(r)>_f} \quad (4.3)$$

In this way, a simple superposition of the different effects is obtained.

To take into account the homogeneous effect, it is necessary to substitute in (4.2) and (4.3) the temperature T'_m to T_m.

An application of the described model has been done in the case of a Candu type cell for which a series of hot loop measurements has been done at Chalk River [8].

The geometrical data of the cell considered are as follows:

Fuel volume (19 UO_2 rodlets)	$V_f = 28.6$ cm²
U effective volume	$V_U = 13.7$ cm²
Coolant volume (D_2O)	$V_c = 19.4$ cm²
Moderator volume (D_2O at 23 °C)	$V_m = 437$ cm²

The value of $\lambda_{\text{reth}}/\lambda_a$ is about 1.4 at $T_c = 250$ °C, so that this case can be considered as intermediate between the two limits mentioned above.

The quantities α and ΔT_n have been calculated by the same temperature definition as used for the interpretation of the experimental data, i.e. by assuming as test event the fission reaction rate ratio Pu^{239}/U^{235}.

The rethermalization effect due to the structural materials and to the O nuclei bound in the UO_2 has been taken into account through (2.8), and the one due to the D nuclei through (2.8′) (D effective mass = 3.6).

The results are:

$$\alpha = \frac{\Delta < T_n >_f}{\Delta T_c} = 0.19$$

$$\Delta T_n = 35 \text{ °C}$$

In fig. 1, together with the experimental points, two theoretical curves are drawn: curve *a*) has been obtained by the application of expression (4.1) or, what practically comes to the same thing, through the combination of (3.12) and (4.3); curve *b*) has been obtained by the determination of the neutron temperature from the spectrum expression (4.2).

The « homogeneous » hardening $T'_m - T_m$ has been taken to be equal to the experimental value of the Chalk River experiments ($T'_m - T_m = 6$ °C). In this way, a comparison between theory and experiment is possible for the quantities which are typically described by the model.

For every T_c value the two curves *a*) and *b*) fix two limits between which the actual neutron temperature should be found.

In fig. 2, together with the maxwellian at the moderator temperature, the rethermalized spectrum for $T_2 = 250$ °C and the hardened one are given by the curves *a*) and *b*) respectively. Fig. 3, again together with the maxwellian at the moderator temperature, shows for the two limit cases *a*) and *b*) of fig. 1, the spectrum which comes out of the combination of hardening and rethermalization at $T_2 = 250$ °C. ■

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riassunto

UN MODELLO SEMPLIFICATO PER LA DETERMINAZIONE DELLO SPETTRO NEUTRONICO TERMICO IN UN ELEMENTO DI COMBUSTIBILE

In quest'articolo viene proposto un modello semplificato per la valutazione dello spettro neutronico termico in un elemento di combustibile, contenente dei materiali moderatori. Benchè complesso, questo problema può essere risolto almeno in prima approssimazione con metodi semplici, purchè l'indurimento dello spettro dovuto all'assorbimento selettivo nel combustibile e la ritermalizzazione dovuta all'interazione con i materiali moderatori siano trattati separatamente. Vengono quindi descritti i metodi usati per valutare separatamente questi effetti ed è proposto un sistema di correlazione dei risultati. È infine presentata e discussa l'applicazione del modello ad una cella, per la quale sono stati effettuati a Chalk River degli esperimenti in circuito caldo.

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