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PROBABILITY TABLES AND GAUSS QUADRATURE ; APPLICATION TO *NEUTRON CROSS-SECTIONS IN THE UNRESOLVED ENERGY RANGE*

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ABSTRACT

The idea of describing neutron cross-section fluctuations by sets of discrete values, called "probability tables", was formulated some 15 years ago. We propose to define the probability tables from moments by equating the moments of the actual cross-section distribution in a given energy range to the moments of the table. This definition introduces PADE approximants, orthogonal polynomials and GAUSS *quadrature. This mathematical basis applies very well to the total* cross-section. Some difficulties appear when partial cross- sections are taken into account, linked to the ambiguity of the definition of multivariate PADE approximants. Nevertheless we propose solutions and choices which appear to be satisfactory. Comparisons are made with other definitions of probability tables and an example of the calculation of a mixture of nuclei is given.

The idea of representing cross-sections by sets of discrete values was first proposed by the Soviets in 1969 [1, 2], and independantly by Leo LEVITT in 1970 [3] ; subsequently Dermott CULLEN and others dealt with various developments and applications of the probability tables [4 to 8].

Basically the American and Soviet ideas are the same. The Americans established the table from the neutron cross-sections $\sigma(E)$ in a given energy range by various means and considered the properties of the tables. The Soviets based the tables on a fit to $\sigma_{x,eff}(d)$, the effective partial cross-sections as a function of the background cross-section ; more importantly they proposed to abandon the concept of "effective cross-section" and to introduce the "probability tables" directly in the neutronic calculation. By doing this they divide every energy group into "sub-groups" ruled by the neutronic equations which classicaly rule the groups, except for scattering (scattering exists between all sub-groups belonging to the same group). The same idea was proposed by D. CULLEN as the "multiband method" [5, 7].

Following these historic origins and in hommage to these precursors we shall use, hereafter and in another paper, the name "probability table" every time we deal with the establishing of the tables and their properties, the name "subgroup method" when we consider the application of these tables to neutronics.

Our basic idea is to generalise, deepen and increase the exactitude of these concepts ; to do so we base the probability tables upon moments : the probability table method is then merely a GAUSS quadrature.

This paper deals with the cross-section probability tables : no problem arises for total cross-section (§2,5), a few difficulties when partial cross-sections are taken into account (§7). We show the improvement in accuracy resulting from our approach (§3) and consider another approach, to be rejected (§4). We compare the tables based on moments with those deduced from $\sigma_{eff}(d)$, as proposed by the soviets and as used by some laboratories (§8). We then give some simple examples of applications, independant of neutronics (mixture of nuclei, §9). More details are given in the report NEARCP-L-294 [9].

1 - PRINCIPLE - The $\sigma$ range is divided into N intervals: 3 in figure 1. To each of these intervals we associate $(p_i, \sigma_i)$: $p_i$ will represent the probability that $\sigma(E)$ will lie within this interval characterized by $\sigma_i$. In mathematical terms:

$$(1-1) \qquad p_i = \frac{\int_{E_i}^{E_s} \delta(\sigma(E), i)\, dE}{E_{sup} - E_{inf}}$$

with : (1-2) $\quad \delta(\sigma(E), i) = 1 \quad$ if $S_{i-1} < \sigma(E) < S_i$
$\qquad\qquad\qquad = 0 \quad$ is not.

Several definitions are possible for $\sigma_i$ such as the median, or an average defined by :

$$(1-3) \qquad p_i\ \sigma_i = \frac{\int_{E_i}^{E_s} \sigma(E)\ \delta(\sigma(E), i)\, dE}{E_{sup} - E_{inf}}$$

The couples $(p_i, \sigma_i)$ will characterize the cross section behaviour in the energy range $(E_{inf}, E_{sup})$ all the more accurately as N, the number of couples (which we shall call the "order" of the table), increases.

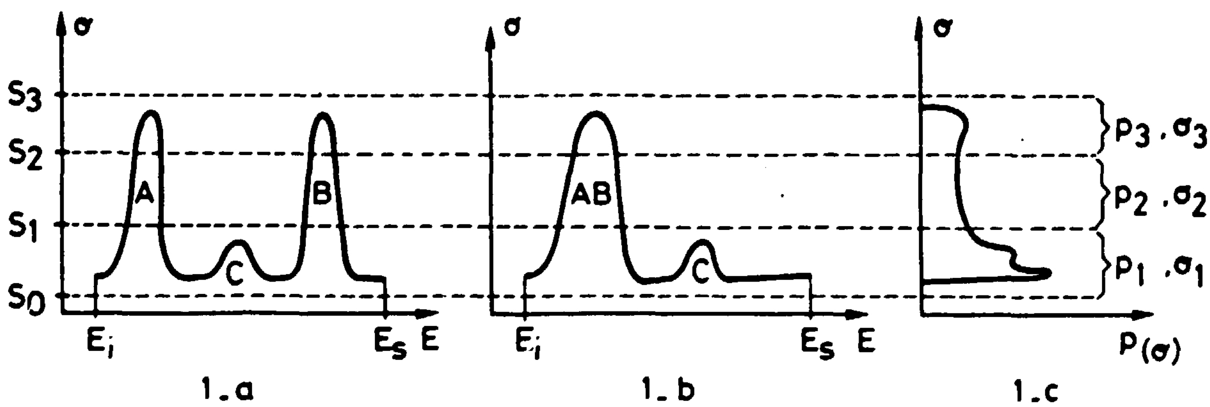



Fig. 1 - Representation of the discretisation of a few resonances. There is no overlap between resonances A, B and C of fig. 1 : $p(\sigma)$ (fig. 1-c) will not change if A, B and C are permuted. Resonances AB of fig. 1-b have the same shape as resonances A and B (which are identical), with twice their width : AB and C of fig. 1-b will provide the same $p(\sigma)$ as A, B and C of fig. 1-a.

It is obvious however that energy information is lost: the table is the same if the resonances of figure 1 are permuted. Furthermore the resonances represented by fig. 1a and 1b will have the same probability table. This has 2 consequences:

- so defined the probability tables imply the statistical hypothesis, i.e. little sensitivity to permutation of resonances (the effects are due to the overlapping of wings) ;
- such a probability table is always associated with the narrow resonance approximation.

Evolution of the American school - Several papers deal with the application of the "multiband method" to neutron transport equations ; the tables are generally "equal probability tables" [5]. Recently CULLEN and POMRANING prescribed the conservation of four averages, from order -2 to order 1 ; in the same paper [7] they concluded that it was "a classical moments problem", but remark that as "in general there is no reason to do otherwise (they) use equal band weights".

The Soviet school - From the very beginning the Soviets accepted the need to calculate $p_i$ and $t_i$, which they do by a least squares method (cf. §8).

The French approach - We choose to define a probability table by equating 2N moments of the $\sigma(E)$ distribution to the same 2N moments of $(p_i, \sigma_i)$, i.e.:

(1-4) $$\mathrm{m}_n \equiv \frac{1}{\Delta E}\int_{\Delta E} \sigma^n(E)\, dE = \sum_{i=1} p_i\, \sigma_i^n \equiv M_n$$

for 2N values of n ; the integral - a RIEMANN integral - can be written as a LEBESGUE integral :

(1-5) $$\mathrm{m}_n \equiv \int_\sigma \sigma^n\, p(\sigma)\, d\sigma$$

figure 1 illustrates this process.

We are then faced with a non-linear system of 2N equations with N couples of unknowns $(p_i, \sigma_i)$. The values n are a priori arbitrary : we choose to have a sequential series of values ranging from I to I+2N-1, where I can be negative (choice justified by 2-1-a) :

(1-6) $$I \leq n \leq I + 2N - 1$$
$$\text{with: } 2 - 2N \leq I \leq 0$$

the limits of I are determined by the requirement that values n=0 and n=1 lie within the series.

2 - PROPERTIES OF THE PROBABILITY TABLE AS A GAUSS QUADRATURE METHOD - How can the system 1-4 be solved? By the following sequence of transformations, written in the simple case I=0 :

(2-1-a) $$F(z) = \int_\sigma \frac{p(\sigma)}{1-z\sigma}\, d\sigma = \int_\sigma p(\sigma)(1 + z\sigma + \ldots + z^k\sigma^k + \ldots)d\sigma$$

(2-1-b) $$= \mathrm{m}_0 + \mathrm{m}_1 z + \ldots + \mathrm{m}_{2N-1}\, z^{2N-1} + \mathcal{R}(z^{2N})$$

(2-1-c) $$= \frac{a_0 + a_1 z + \ldots + a_{N-1} z^{N-1}}{1 + b_1 z + \ldots + b_N z^N} + \mathcal{R}'(z^{2N}) \equiv \frac{P_{n-1}(z)}{Q_n(z)} + \mathcal{R}'(z^{2N})$$

(2-1-d) $$= \frac{P_{n-1}(z)}{\prod_{i=1}^N (1 - \frac{z}{z_i})} + \mathcal{R}'(z^{2N}) = \sum_{i=1}^N \frac{\omega_i}{1 - \frac{z}{z_i}} + \mathcal{R}'(z^{2N})$$

The stipulation $\mathrm{m}_n = M_n$ allows 2-1-b to be written:

(2-2-a) $$F(z) = M_0 + M_1 z + \ldots + M_{2-1} z^{2N-1} + R(z^{2N})$$

(2-2-b) $$= \sum_{i=1}^N p_i(1 + \sigma_i z + \sigma_i^2 z^2 + \ldots + \sigma_i^{2N-1} z^{2N-1}) + R(z^{2N})$$

(2-2-c) $$= \sum_{i=1}^{N} \frac{p_i}{1 - \sigma_i \; z_i} + R' \; (z^{2N})$$

then by identifying 2-1-d and 2-2-c :

(2-3-a) $p_i = \omega \qquad\qquad \sigma = 1/z_i$

If $I \neq 0$ we obtain, by the same process :

(2-3-b) $\rho_i = \sigma_i^I \qquad\qquad \sigma_i = 1/z_i$

The process described by equations 2-1 calls for a few comments:

PADE approximant. The transition from 2-1-b to 2-1-c is the transformation of a series into a PADE approximant $P_{N-1}/Q_N$. This transformation exactly describes the first 2N terms of 2-1-b, the rest being modified in such a way that, very generally :

(2-4) $$\mathcal{R}' \; (z^{2N}) \ll R'(z^{2N})$$

The equations ruling this transformation are :

(2-5-a)
$$\begin{aligned} a_0 &= m_0 \\ a_1 &= m_1 + m_0 \; b_1 \\ &\text{- - - - - - - - - - -} \\ a_{N-1} &= m_{N-1} + m_{N-2} \; b_1 + \text{- - - - - - - - - - -} + m_0 \; b_{N-1} \end{aligned}$$

(2-5-b)
$$\begin{aligned} 0 &= m_N + m_{N-1} \; b_1 + \text{- - - - - - - - - - -} + m_1 \; b_{N-1} + m_0 \; b_N \\ 0 &\text{ - - - - - - - - - - - - - - - - - - - - - - -} \\ 0 &= m_{2N-1} + m_{2N-2} \; b_1 + \text{- - - - - - - - - - - - - - -} + m_{N-1} \; b_N \end{aligned}$$

The resolution of the linear system 2-5-b provides the values of $b_n$ which, reported in 2-5-a, immediately give the values of $a_n$.

Calculation of the Roots of $Q_N$ - Many routines compute the roots of a polynomial ; the properties of these roots are examined in 2-2. Here we shall merely note that no double roots are present as long as $p(\sigma)$ is, at least partly, a continuous distribution. Theoretically we have multiple roots only when we want to describe a distribution consisting of N DIRAC functions (i.e. a probability table of order N) by another of order N' with $N' > N$ : it is possible to reduce but not to increase the order of a probability table.

Calculation of the weights $\omega_i$ - No difficulty arises in the absence of multiple roots.

Properties of the probability tables - Equations 2-5-b are equivalent to the assessment :

$$\mathcal{I}_n = \int_\sigma \sigma^n \; p(\sigma) Q_N(\sigma) \; d\sigma = 0 \qquad\qquad \text{for } n < N$$

i.e. $\sigma^n$ and $Q_N(\sigma)$ are orthogonal (relative to the probability distribution $p(\sigma)$); hence $Q_N$ and $Q_{N'}$, $N' \neq N$, are orthogonal. It can also be easily shown that, whatever may be a formal expansion of $f(\sigma)$ valid on the support of $\sigma$:

$$\mathcal{I} = \int_\sigma f(\sigma) \; p(\sigma) \; d\sigma \# \sum_i p_i \; f(\sigma_i)$$

As an implicit fact we introduce, by means of PADE approximants, the orthogonal polynomials generated by $p(\sigma)$ and the GAUSS quadrature. The aim of this paper is not to expose this theory : the reader may refer to many references [10 to 14]. We shall merely report a few results of interest for our purpose.

Roots of $Q_N$ - The N roots $\sigma_i$ are real and on the support of $\sigma$. Every one of the N roots of $Q_N$ lies within one of the N intervals defined by the N+1 roots of $Q_{N+1}$.

Positivity of $p_i$ ($\equiv \omega_i / \sigma_i^N$) - When $p(\sigma)>0$, whatever $\sigma$ : $p_i > 0$. These discrete weights $p_i$ are sometime called "CHRISTOFFEL numbers".

Separation of bands and roots - When $p(\sigma)>0$, unique values $S_i$ exist such that:

$$
(2\text{-}6)\qquad
\begin{aligned}
&\int_L^{S_1} p(\sigma)\, d\sigma = p_1\\
&\int_{S_1}^{S_2} p(\sigma)\, d\sigma = p_2\\
&- - - - - - - - - - -\\
&\int_{S_{N-1}}^{G} p(\sigma)\, d\sigma = p_N
\end{aligned}
$$

L and G being the lowest and highest values of $\sigma$ (i.e. the bounds of the support of $\sigma$). These values $S_1$, $S_2$, ... are such that :

$$
(2\text{-}7)\qquad L < \sigma_1 < S_1 < \sigma_2 < S_2 \ldots < \sigma_{N-1} < S_{N-1} < \sigma_N < B
$$

and the multiband interpretation, as illustrated by fig. 1, is then physically meaningful.

Separation of bands of order N and (N+1) - If $S_{i,N}$ denote the limits defined by (2-6) for the N-th table, then :

$$
(2\text{-}8)\qquad L < S_{1,N+1} < S_{1,N} < S_{2,N+1} < S_{2,N} \ldots < S_{N,N+1} < S_{N,N} < S_{N+1,N+1} < G
$$

Quadrature convergence - The quadrature is stable and convergent.

Consistency of moments - STIELTJES'moment problem always has a solution if the series of moments satisfies some conditions, such as :

$$
(2\text{-}9)\qquad \sum_{i=0}^{n} (-)^i C_n^i \mathfrak{m}_{i+k} > 0
$$

or, with the HANKEL determinant :

$$
(2\text{-}10)\qquad \Delta_{k,n} = \begin{vmatrix} \mathfrak{m}_k & \mathfrak{m}_{k+1} & ----- & \mathfrak{m}_{k+n} \\ \mathfrak{m}_{k+1} & \mathfrak{m}_{k+2} & ----- & \mathfrak{m}_{k+n+1} \\ - - & - - & ------ & - - - \\ \mathfrak{m}_{k+n} & \mathfrak{m}_{k+n} & & \mathfrak{m}_{k+2n} \end{vmatrix} > 0
$$

This implies strong restrictions on the possible values of high order moments : typical examples show that a $0.5\ 10^{-6}$ relative modification of moments of 10th or 11th order in a series of 12 positive moments (defining a 6th order table) can provide negative values of $p_i$, or values of $\sigma_i$ outside the range of $\sigma(E)$. Any algebra with moments then requires an accuracy depending on the order, but currently better than $10^{-8}$.

Remark - Formally the reported properties are established for a series of positive moments, ranging from 0 to 2N-1. The extension to negative moments is obvious : we just have to lay pose:

$$q(\sigma) = \sigma^{-I} \, p(\sigma)$$

and deal with the new probability distribution $q(\sigma)$ and only the positive moments. All the properties reported for $\sigma_i$ and $S_i$ are then valid.

3 - TREATMENT OF CULLEN'S EXAMPLES - In order to demonstrate the interest of the multiband method Dermott CULLEN taken theoretical examples of which exact analytical solutions could be determined, thus providing a reference.

First example - D. CULLEN considered a unidirectional source of neutrons incident on a purely absorbing medium. He assumed the cross section probability as given by:

$$(3\text{-}1) \qquad \begin{array}{ll} p(\Sigma) = 0.15 - 0.006\ (\Sigma-10)^2 & \text{for} \leqslant \Sigma \leqslant 15 \\ p(\Sigma) = 0 & \text{otherwise.} \end{array}$$

This author calculated the exact analytical solution expressing the neutron flux as a function of depth, and computed the results with the equal probability multiband method.

Resuming his calculations with his method, we obtained his results. We treated the same problem with our probability tables which, it will be remenbered, are a function of two parameters : order N and value I of first-order moment. Some results are shown on fig. 2 where a great improvement in accuracy is observed.

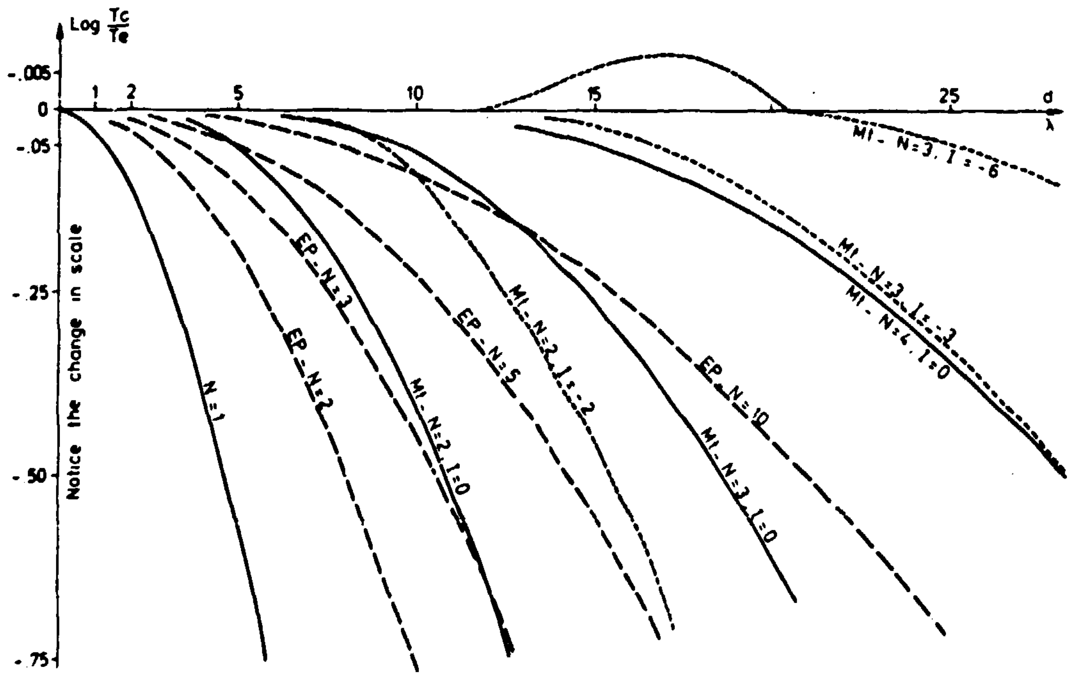



Fig. 2 - CULLEN'S first example. Ratio of the transmission calculated with probability tables Tc, to the exact analytical value Te. The penetration d is expressed in mean free path unit.

EP stands for "equiprobable" tables, Mt for tables based on moments, either positive only (full line, I=0), or positive and negative (dotted line, I<0).

Second example - CULLEN and POMRANING again considered a unidirectional flux of radiation impinging perpendicularly on a half-space medium, without re-emission of secondary particles. The problem is the same as previously, with a different law p(E). The results given are obtained with a two-band method, defined as explained here in §1 : this method is then strictly equivalent to our moments method, with N=2, I=-2.

4 - THE EQUIPROBABLE MOMENTS METHOD OR TCHEBICHEV METHOD - The moments method used to define probability tables is then very coherent and has a strong (and rich) mathematical support, but do other possibilities exist?

Amongst other possible methods is the TCHEBICHEV integration formula [15]: the $x_i$ values are calculated from the equality of N moments $\mathfrak{m}_n$ and $M_n$, the probability $\sigma_i$ being a constant :

$$(4\text{-}1) \qquad p_i = 1/N$$

This method is less accurate, but may have some advantages. However we lack any kind of mathematical theory justifying "good" properties for the $\sigma_i$ and it is easy to find examples proving the contrary :

a) for $p(x) = 1$ in the internal $(-1,+1)$
$= 0$ elsewhere.

values of $x_i$ lie outside the range $(-1,+1)$ for n=8 and for n>9 ;

b) for $p(x) = e^{-x}$ $x > 0$
$= 0$ $x < 0$

the roots $x_i$ are complex for $N = 3$.

We therefore conclude that this method cannot be applied to describe the neutron cross-section behaviour.

5 - NEGATIVE MOMENTS - It is clear that the accuracy will improve as N increases but what can be said of I, the order of the first moment taken into account ? Examination of figure 2 provides a first answer : accuracy appears to improve as I decreases (in the algebraic sense). This is due to the fact that the CULLEN examples are deep-penetration problems ; a careful examination of numerical results shows that accuracy decreases as I decreases for small penetrations.

In order to study this problem we calculated as an example the effective cross-section of a nucleus :

- directly, with formula 5-1 ; this provides the reference ;
- by probability tables, with formula 5-2, to various orders.

$$(5\text{-}1) \qquad \sigma_{eff,ref}(d) = \frac{\int \frac{\sigma(E)}{\sigma(E)+d}\, dE}{\int \frac{1}{\sigma(E)+d}\, dE} \qquad\qquad (5\text{-}2) \qquad \sigma_{eff,N,I}(d) = \frac{\sum_{i=1}^{N} \frac{p_i\, \sigma_i}{\sigma_i + d}}{\sum_{i=1}^{N} \frac{p_i}{\sigma_i + d}}$$

$$(5\text{-}3) \qquad \epsilon_{N,I}(d) = \mathrm{Log}\, \frac{\sigma_{eff,N,I}(d)}{\sigma_{eff,ref}(d)}$$

The error is given by 5-3, the probability table $(p_i, \sigma_i)$ being defined by 2N moments ranging from I to I+2N-1. The chosen nucleus was $^{238}U$ between 4250 and 4750 eV, the resonance parameters ("s" wave only) being generated by the regularised method [15] with the following parameters (ENDF-B-4) :

$R = 9.184$ fm $\qquad \bar{D}_{\ell=0} = 19.98$ eV
$S_o = 1.05\ 10^{-6}$ $\qquad \Gamma_\gamma = 0.0235$ eV.

Results were obtained for T = 0 K (unrealistic, but reinforced effects), T = 300 K and T = 1500 K. The general behaviour is the same and is illustrated by figure 3 in the case T = 300 K, for 3 dilutions d :

- when d is large the accuracy is provided by positive moments ;
- when d is small the accuracy is provided by negative moments ;
- for medium values (d = 20 barns) the accuracy depends on N only.

From these results we defined a "standard" choice : I=1-N

For any particular application the user can reduce the order of the table with emphasis on negative or positive moments.

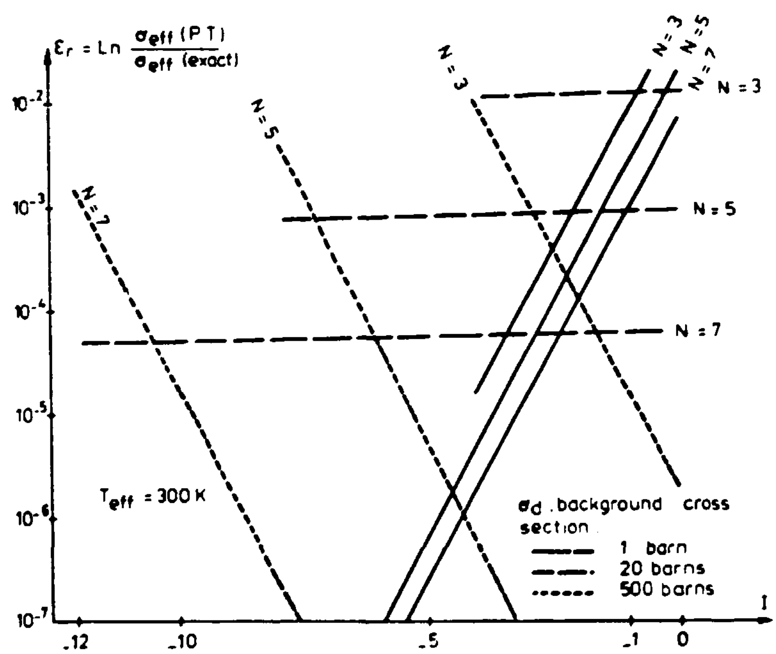



Fig.3 - Relative error on $\sigma_{t,eff}$ calculated with probability tables for various values of N (order of the table) and I (lowest order of the moments taken into account - I<0).

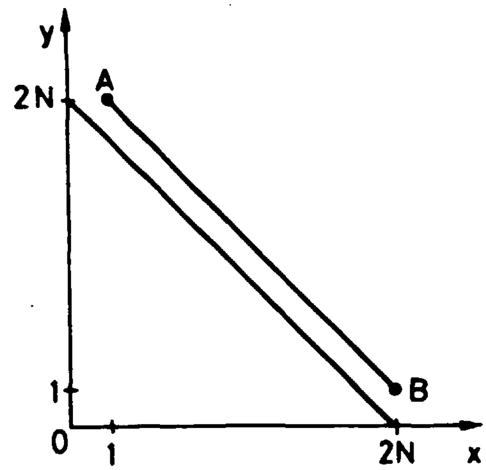
6 - PROBABILITY TABLES WITH PARTIAL CROSS-SECTIONS - The mathematical theories of PADE approximants, of orthogonal polynomials and of the GAUSS quadrature are well established in the one-variable case. This is not longer true when we consider partial cross-sections, i.e. a multivariate problem. The difficulties appear from the first step : the PADE approximant.

Multivariate PADE approximants - Equations 2-1-b and 2-1-c form the general, unambiguous and universally accepted definition of one variable PADE approximants. On the contrary no unique canonical definition of multivariate approximants exists (cf [17]). We give as an example the CHRISHOLM proposition [12].

This author proposed for a 2 variable (N,N) approximant:

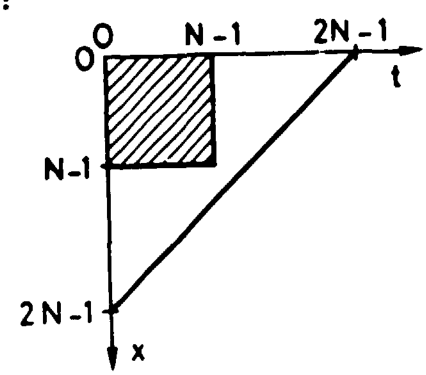
$$(6\text{-}1)\quad \begin{cases} P_N = \sum_{i=0}^{N} \sum_{j=0}^{N} a_{ij}\, x^i\, y^j \\ Q_N = \sum_{i=0}^{N} \sum_{j=0}^{N} b_{ij}\, x^i\, y^j \end{cases}$$

with $b_{00}=1$ ; the determination of all values $a_{ij}$ and $b_{ij}$ requires $2(N+1)^2-1$ elements of data: CHRISHOLM proposes to keep the triangle (0-2N-2N), which provides (N+1)(2N+1) moments to be completed by N values taken among the 2N values of AB. Whatever choice is made, it is clearly arbitrary.




Attemps to obtain a secondary distribution for partial cross sections - On a subjective basis it seems desirable to associate partial cross-section distributions to every discrete total cross-section value. We tried several methods, without success ; for example the following solution was considered (t stands for $\sigma_t$ ; x for $\sigma_x$, a particular partial cross-section) :

$$\begin{array}{cc|ccc|} & & q_1 & q_2 & q_3 \\ & & x_1 & x_2 & x_3 \\ \hline p_1 & t_1 & w_{11} & w_{12} & w_{13} \\ p_2 & t_2 & w_{21} & w_{22} & w_{23} \\ p_3 & t_3 & w_{31} & w_{32} & w_{33} \\ \hline \end{array}$$




The probability table for total cross-section is defined by 2N moments on axis t. To define the values $x_j$ and $w_{ij}$ we needed N items of information (for $x_j$) and N(N-1) for $w_{ij}$ (since $\Sigma^j w_{ij} = p_i$ is already known), i.e. $N^2$ moments outside the t axis. These can be provided by 2N-1 moments on the x axis, and by the $(N-1)^2$ values of the hatched square. The cross-probability table can then be clearly and unambiguously defined.

However we cannot be sure that $w_{ij} > 0$, nor physically interprete the case $x_j > t_i$ with $w_{ij} \neq 0$ (i.e. a non zero, possibly positive, probability of having a partial cross section greater than the total cross-section). We used this method for a while and such contradictions arose (with the fact that absolute non-physical values of $w_{ij}$ were small).

Uselessness of secondary probability tables - However the search for secondary probability tables is a false problem in neutronics since the partial cross sections always appear linearly in expressions, i.e. with the general form :

$$(6\text{-}2)\qquad I = \int x\, f(t)\, dE$$

Hence even if a convenient secondary table were available with weights $w_{ij}$, we would have :

$$(6\text{-}3)\qquad I = \sum_i f(t_i) \sum_j w_{ij}\, x_j = \sum_i f(t_i)\, x_i$$

Thus the knowledge of a single value $x_i$, associated with $t_i$, is all we require.

Definition of discrete partial cross-section values - As in the case of the total cross-section we defined the discrete values $x_i$ by equalizing N moments implying the partial cross-section:

(6-4) $$\mathscr{P}_{x,p} \equiv \frac{1}{\Delta E} \int_{\Delta E} x\, t^n\, dt = \sum_i p_i\, x_i\, t_i^n \equiv P_{x,n}$$

Internal consistency of probability tables - By applying this process to every partial cross-section we define values of $s_i$ (scattering), $c_i$ (capture), $f_i$ (fission), ... and the problem is one of consistency with the total cross-section, i.e.:

(6-5) $$t_i = s_i + c_i + f_i + \dots = \sum_x x_i \quad ?$$

This is automatically ensured by the method with a proper choice of moments order as shown below in the case of a second-order table. We have:

(6-6) $$\begin{cases} \int t^m\, dE = \int t^{m-1} \sum_x x\, dE \\ \int t^n\, dE = \int t^{n-1} \sum_x x\, dE \end{cases}$$

Written in terms of probability tables :

(6-7) $$\begin{cases} p_1\, t_1^m + p_2\, t_2^m = p_1\, t_1^{m-1}\, \Sigma\, x_1 + p_2\, t_2^{m-1}\, \Sigma\, x_2 \\ p_1\, t_1^m + p_2\, t_2^n = p_2\, t_1^{n-1}\, \Sigma\, x_1 + p_2\, t_2^{n-1}\, \Sigma\, x_2 \end{cases}$$

Multiplying the second equation by $t_2^{m-n}$ and substracting it from the first, we obtain :

(6-8) $$p_1 (1-(\frac{t_1}{t_2})^{n-m})\, t_1^m = p_1\, (1-(\frac{t_1}{t_2})^{n-m}) t_1^{m-1}\, \Sigma_x\, x_1$$

hence, if $m \neq n$ and $t_1 \neq t_2$ (non-degenerated table) ;

(6-9) $$t_1 = \Sigma_x\, x_1$$

Generalizing this calculation to higher orders we arrived at the following conclusion: in order to obtain the internal consistency of probability tables, as defined by 6-5, we have to associate the 2N successive moments $\mathfrak{M}_n$ of the total cross section, with order ranging from I to I+2N-1, to the N moments $M_n$ as defined by 6-4, with :

- either consecutive orders ranging from J to J+N-1, with :

  $I - 1 < J < I+N$

several solutions are possible ;

- or orders varying by 2 units, from J to J+2N-2 ; two possible solutions exist, only one if 0-th order is required for normalisation.

7 - CHOICE OF "PARTIAL" MOMENTS - Let us first consider the case of sequences of moments with $\delta n=1$ and, in § 7-3, the case $\delta n=2$.

7.1 - Accuracy provided by the tables - Figure 4 represents a schematisation of the accuracy obtained on $\sigma_{c,eff}(d)$ with tables (N=7,I,J), at T=0 K, for d=1 barn and d=500 barns. We also considered the quadratic sum of $\varepsilon(d=1)$ and $\varepsilon(d=500)$ and concluded that the best choice is : $J=-N/2$

Fig.4 - Relative error on $\sigma_{c,eff}$ calculated with probability tables for various values of I (lowest value of the total cross-section moments) and of J (lowest value of the "partial cross- section moments).

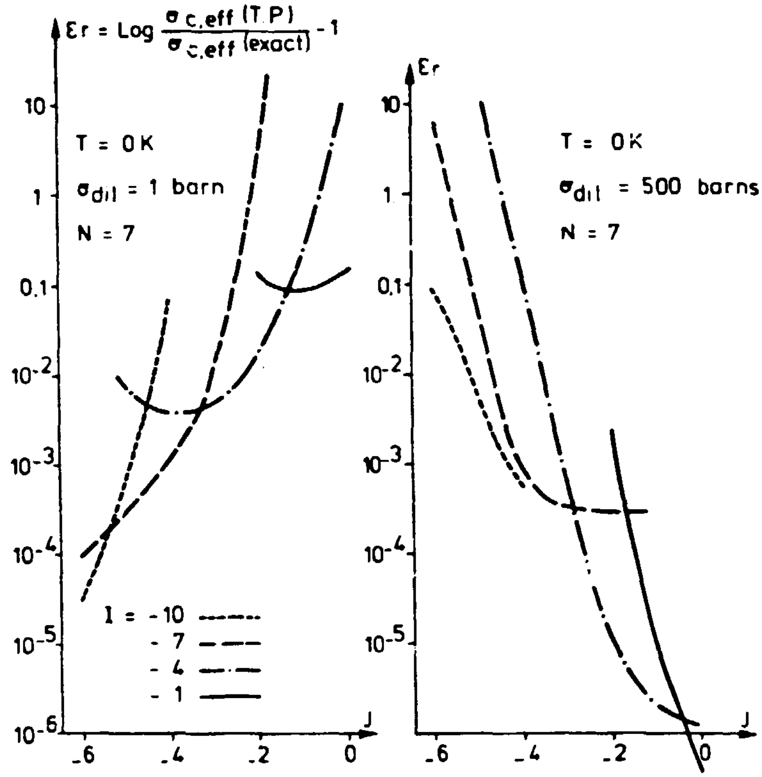



Figure n°4

7.2 - Positivity of discrete partial cross-section values - The problem is : do the values $x_i$ lie on the support of x(E) ? There is no mathematical background to maintain such a conclusion and we obtained many examples proving it to be false.

Some results are given concerning the 4 independant cases defined in §5. For simplicity we concentrate only on the counting of negative $x_i$'s values. We considered every order from N=2 to N=7, for all possible values of I and J. Table 1 represents results for the capture cross section with N=6. This table, and similar tables for other values of N, show that the choice J=(I-1)/2 defines a valley containing very few cases of negative values.

Table 1 - Number of negative partial cross-sections values obtained for 6-th order probability tables. The broken lines delimit the coherent area (cf.§6) outside which are many negative values. Bold types correspond to the recommanded choice :

J = (I-1)/2

The square represents the standard choice :

I = 1-N J = - N/2

| J = -5 | -4 | -3 | -2 | -1 | 0 | I = |
|---|---|---|---|---|---|---|
| 0 | 0.2 | 4 | 5 | 6 | 6 | -10 |
| 0 | 0 | 1.5 | 4 | 5 | 6 | -9 |
| 0 | **0.2** | 0.2 | 2 | 4 | 4.5 | -8 |
| 0 | **0** | 0.5 | 0.2 | 2 | 4 | -7 |
| 0 | 0 | **0.2** | 0.5 | 0.5 | 2 | -6 |
| 0 | 0 | $\boxed{0}$ | 0 | 0.2 | 1 | -5 |
| 1 | 0 | 0 | **0** | 0 | 0.2 | -4 |
| 3 | 1 | 0 | **0.2** | 0.7 | 0.5 | -3 |
| 4 | 2.7 | 0.7 | 0.2 | **1** | 1 | -2 |
| 4 | 4 | 2 | 0 | **0.2** | 1 | -1 |
| 5 | 4 | 3.7 | 0 | 0 | **0** | 0 |

We have also considered the behaviour of the probability tables around the standard choice I=1-N, J=-N/2. Examination of these results shows that negative values, if any, are very small, and next to at least one table without negative partial cross-section value. We can therefore propose the following alternatives:

- either to accept values of discrete partial cross sections outside their support (i.e., in practice, to keep negative values) ;
- or to search for a "good" table in the vicinity of the standard choice.

7.3 - Sequences of partial moments with $\delta n = 2$

Accuracy - The best accuracy is less by a factor 10 to 1000 than that provided by tables with $\delta n = 1$.

Positiveness of $\sigma_{x,i}$ - Our purpose was to check whether for some unknown reason every value $\sigma_{x,i}$ lay within its support. Such is not the case: the number of negative values is at least as great as for the case $\delta n = 1$.

Conclusion - From this we conclude that the system of partial moments with $\delta n = 2$ presents no interest compared to the more classical choice $\delta n = 1$.

8 - PROBABILITY TABLES : BASIC DATA OR INTERPOLATORY METHOD ? - From the very begining the Soviets proposed to determine the tables by fitting the effective partial cross section values calculated for several values of the background cross-section $d_j$:

$$(8\text{-}1) \qquad \sigma_{x,eff}\,(d) = \frac{\sum_i \frac{p_i x_i}{t_i + d_j}}{\sum_i \frac{p_i}{t_i + d_j}}$$

The knowledge of effective cross-section values for at least 2N values of $d_j$ allows the determination of a probability table. Basically this is the method used in various laboratory as the "subgroup method" [18]. How does it compare with the probability table based on moments ?

We compared results obtained by these two methods, referring the effective cross sections to the exact values obtained by direct integration. Our test case was $^{238}U$ at 300 K between 4400 and 4600 eV.

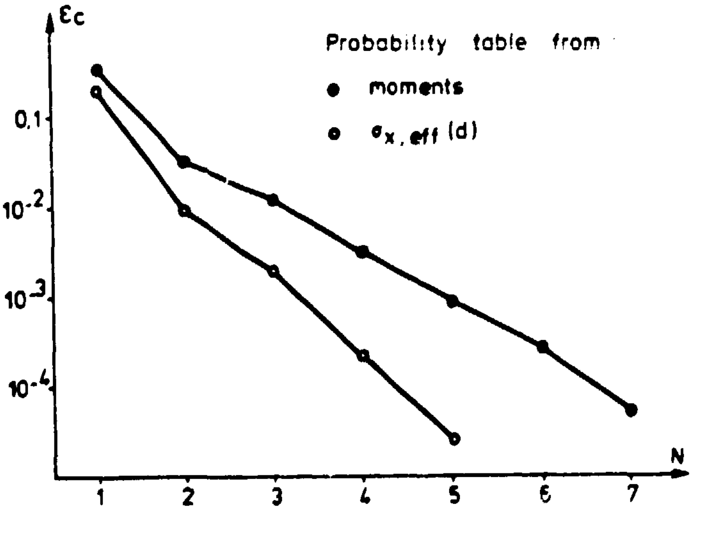
The values of the effective cross sections were calculated for 41 dilutions $d_j$, ranging from d=1 barn to $d=10^4$ barns, and for $d_{42}=10^7$ barns. A least square fitting of $\sigma_t(d_j)$, $\sigma_s(d_j)$ and $\sigma_c(d_j)$ allows the determination of probability tables of order ranging from 1 to 5 and of a quadratic average of errors :

$$s_x^2 = \left\langle \left(\frac{\sigma_{x,eff}(P.T)}{\sigma_{x,eff}(exact)} - 1\right)^2 \right\rangle$$

The determination of probability tables from moments calculated with the same data allows the calculation of another average quadratic error.

Comparison of results is plotted in figure 5 for capture. It appears that the error is smaller in the former case: this is natural since the probability tables are than adjusted to the data on which they are checked.

Fig.5 - Values of $\varepsilon_c$, the error on $\sigma_{c,eff}$, as a function of N, the order of the table.



If the aim is merely to use the probability tables as an interpolation method over $\sigma_d$ the values deduced from $\sigma_{x,eff}(d_j)$ are to be preferred, but such tables are dependant on the $\sigma_{x,eff}$ calculation method and on the least squares method.

On the contrary the tables deduced from moments are basic data, independant of any application. They are more general, and can be used for quadrature.

9 - CALCULATION OF MIXTURES OF NUCLEI - The reactor physicist is always faced with mixtures of nuclei, the ratios of which may vary. The definition of probability tables from moments offers an easy way to calculate the nuclear property of any mixture.

This is obvious in the case of probability tables based only on the positive moments: we have, for the mixture of two nuclei $t_1$ and $t_2$, with ratio $\alpha$ and $\beta$ ($\alpha+\beta=1$):

$$(9\text{-}1)\quad \begin{cases} \mathbf{m}_n = \int_{\Delta E} t^n \frac{dE}{\Delta E} = \int (\alpha\, t_1 + \beta\, t_2)^n \frac{dE}{\Delta E} \\ \quad = \sum_{i=0}^{n} C_n^i\, \alpha^i\, \beta^{n-i} < t_1^i\, t_2^i\, t_2^{n-i} > \end{cases}$$

With the statistical assumption:

$$(9\text{-}2)\quad < t_1^i\, t_2^{n-i} > = < t_1^i > < t_1^{n-i} > = \mathbf{m}_{1,i}\, \mathbf{m}_{2,n-i}$$

we obtain:

$$(9\text{-}3)\quad \mathbf{m}_n = \sum_{i:0}^{n} C_n^i\, \alpha^i\, \beta^{n-i}\, \mathbf{m}_{1,i}\, \mathbf{m}_{2,n-i}$$

Similar expressions stand for the partial cross-sections.

The knowledge of the moments of every nucleus immediately provides the moments of their mixture, then the probability table characterizing this mixture.

But how can we deal with the probability tables established from positive and negative moments ? Two methods may be considered:

- the negative moments of the mixture are calculated by a GAUSS quadrature:

$$(9\text{-}4)\quad \int t_1^m (E)\, t_2^n (E) \frac{dE}{\Delta E} = \sum_{i,j} p_{1,i} t_{1,i}^m p_{2,j} t_{2,j}^n$$

- the probability tables are treated as "positive" probability tables, and the table for the mixture is calculated as previously. The basis of this approach is that the infinite series of positive moments describes unambiguously the table considered, even when established with some negative moments, then that the composition of the positive moments includes the information introduced by the negative moments.

Numerical verification - To check these principles we randomly generated cross-sections for 2 nuclei, calculated their probability tables and computed directly the mixture of these 2 nuclei and its effective cross sections; we also computed the probability table of the mixture from the 2 elementary tables, and from this deduced other effective cross-section values.

These two sets of values always differ since many sets of resonance parameters will give the same set of moments (in fig.1, permutation of resonances or slight shifts in energies will not modify the table). The composition of the 2 elementary probability tables implicitely integrates over all the possible sets of parameters providing the same moments.

To compensate for this effect we study 32 random cases of a mixture of $^{238}U$ (50%) and $^{239}Th$ (50%) between 5985 and 6485 eV in the following ways:

a) computation of $\sigma_{x,eff}(d)$ by direct integration of $\frac{1}{2}(\sigma_U(E)+\sigma_{Th}(E))$;

b) composition of elementary probability tables established from positive moments;

c) composition of elementary tables established from positive and negative moments (standard choice), by 2 methods:

1 - GAUSS quadrature;

2 - composition of positive moments;

d) composition of elementary tables established from $\sigma_{x,eff}$ by a least squares method (26 values of $d_j$), by 2 methods:

1 - GAUSS quadrature;

2 - composition of positive moments.

We also define a "reference" obtained by extrapolating results taken from high order probability tables (5 to 9).

As an example, table 1 presents one case of probability tables involved in the calculation: the 3 tables presented describe the same data (the first random case of $^{238}U$) but are established by 3 different methods.

Tableau 2 - Example of probability table; order 4, for $^{238}U$
(6235 $\pm$ 250 eV, 300 K)

| Established by moments method: positive moments I=0, J=0 | | | Established by moments method: positive and negative moments I=-3, J=-2 | | | from $\sigma_{x,eff}(d_j)$ (26 values of $d_j$ from 1 barn to $10^7$ barns) | | |
|---|---|---|---|---|---|---|---|---|
| p | $\sigma_t$ | $\sigma_t$ | p | $\sigma_t$ | $\sigma_c$ | p | $\sigma_t$ | $\sigma_c$ |
| 0.8181 | 10.888 | 0.522 | 0.1075 | 6.310 | 0.244 | 0.1704 | 7.069 | 0.220 |
| 0.1482 | 30.967 | 2.644 | 0.7716 | 12.321 | 0.627 | 0.7042 | 12.740 | 0.682 |
| 0.0287 | 80.033 | 3.749 | 0.1069 | 43.062 | 3.679 | 0.1050 | 39.021 | 3.409 |
| 0.0044 | 134.811 | 3.745 | 0.0140 | 114.310 | 2.838 | 0.0204 | 103.882 | 3.305 |

Figure 6 represents the error on $\sigma_{c,eff}$ resulting from the composition of 2 4-th or 6-th order elementary probability tables established from moments for a 1 barn dilution.

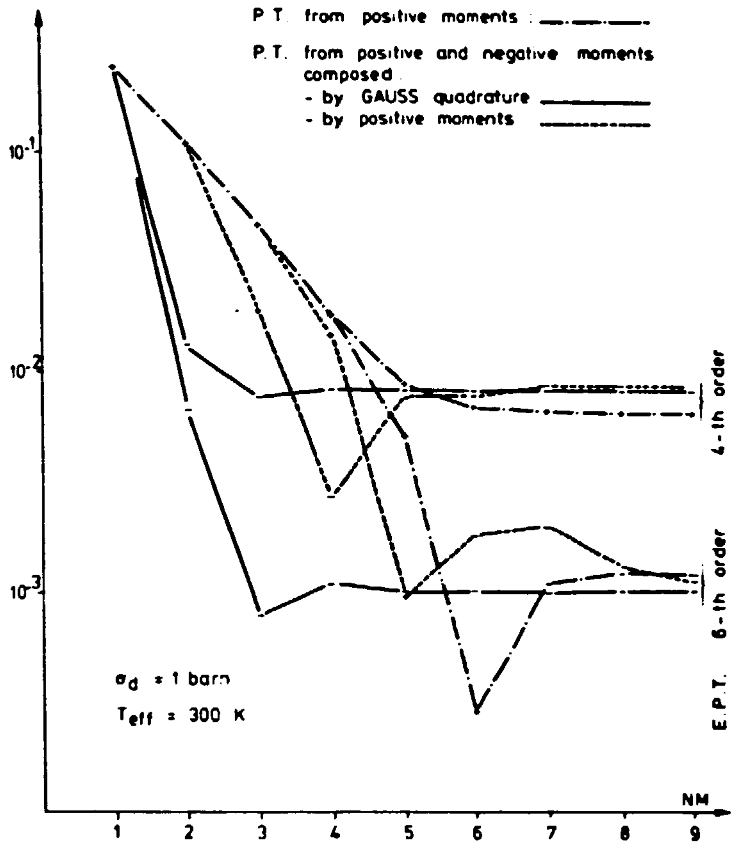



Fig.6 – Accuracy on $\sigma_{c,eff}$ (1 barn) for the mixture of 2 nuclei calculated by composition of probability tables. The elementary tables are 4-th or 6-th order. NM is the order of the probability table of the mixture.

A GAUSS quadrature, with tables established from positive and negative moments, gives the best results and the order NM can be reduced to 3.

Table 3 give the $\sigma_{c,eff}(d)$ values obtained by the various methods described previously.

Table 3 – Mixture of 2 nuclei: Values of $\sigma_{c,eff}(d)$ from different tables established by different methods: N is the order of elementary tables, N' the order of the table for the mixture. The results are the average of 32 cases.

| method | orders N,N' | dilution 1 b. | 20 b. | 500 b. |
|---|---|---|---|---|
| reference | | 0.71680 | 0.80086 | 0.89731 |
| a | | 0.71611 ± 0.0223 | 0.80048 ± 0.0202 | 0.89733 ± 0.0181 |
| b | | 0.74984 ± 0.0170 | 0.80740 ± 0.0164 | 0.89731 ± 0.0177 |
| " | 6-5 | 0.72040 ± 0.0161 | 0.80097 ± 0.0163 | 0.89731 ± 0.0177 |
| c1 | 4-3 | 0.71138 ± 0.0158 | 0.79940 ± 0.0164 | 0.89732 ± 0.0177 |
| " | 6-3 | 0.71624 ± 0.0158 | 0.80241 ± 0.0162 | 0.89736 ± 0.0177 |
| d1 | 4-4 | 0.72152 ± 0.0158 | 0.80086 ± 0.0163 | 0.89727 ± 0.0177 |
| d2 | 4-4 | 0.71687 ± 0.0159 | 0.79992 ± 0.0163 | 0.89724 ± 0.0177 |
| Constant moments fluctuation | | ≈ 0.0157 | ≈ 0.0121 | ≈ 0.0038 |

The "constant moments fluctuation" is the fluctuation on $\sigma_{c,eff}$ for a constant set of moments. It is estimated by a quadratic substraction of errors (case a minus case b).

This table shows that no problem arises for large dilutions (positive moments taken into account are always sufficient). It also shows the good results obtained with tables established from $\sigma_{eff}(d_j)$, despite the lack of theoretical justification for their use in combination of moments.

CONCLUSION - We have shown that the "probability tables" established from moments are merely those required by the GAUSS quadrature, which allows these tables to be used for the complex calculations encountered in neutronics. According to our experience two difficulties remain:

- one concerning the calculation of mixtures of nuclei directly from tables: this is shown to be possible, but some mechanisms are not fully controled. The number of parameters involved and the absence of reference complicate the study and we have considered a theoretical model; this work has to be pursued in greater depth;
- mainly the extension to non-statistical cases (low-energy cross-sections). We have considered these problems but obtained no definite answer; our present tendency is to introduce cross-probability tables containing only the departure from statistical case.

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