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EVALUATED DATA LIBRARIES

A COMPARATIVE STUDY OF THE PROPOSED USSR FORMAT AND THE UKAEA FORMAT

Pierre Ribon
Centre d'Etudes Nucléaires, Saclay

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EVALUATED-DATA LIBRARIES

A comparative study of the proposed USSR format and the UKAEA format

Pierre RIBON
Centre d'Etudes Nucléaires, Saclay

Reactor physicists need "evaluated" nuclear data, i.e. data forming a coherent body of information which an expert - the evaluator - recommends as the best possible estimation in the light of the experimental results and the available theories.

At the same time, using electronic computers, these reactor physicists are performing calculations of increasing precision and they want the information needed for these calculations to be presented in strictly coded forms.

To meet these requirements various formats for evaluated data libraries have been developed during the last eight years and some are still being developed.

We shall study two of these formats:

- The format proposed by K. Parker in 1963-1965 [1], which we shall refer to as the UKAEA format;
- The format proposed by V.E. Kolessov and M.N. Nikolaev [2], which we shall call the USSR format.

That we are familiar with this latter format is due largely to the English translation prepared by A. Lorenz of the IAEA in Vienna, to whom we wish to express our thanks. The present study is based on this translation. The USSR format resembles the UKAEA format.

The exchange of evaluated data is rendered difficult by the existence of these different formats: completely automatic translation of an evaluation from one format to another is not possible. A large number of formats means that more translations have to be made, which in turn means a loss of time and no advantage for anybody.

For this reason, and at the suggestion of the IAEA, we have prepared this report in which we study the differences between the two formats, trying in particular to bring out the differences which would be an obstacle in automatic translation.

We shall start by reviewing the differences in the information content.

I. PHYSICAL CONTENT OF THE USSR LIBRARY

This library provides for the same information as that which the UKAEA library contains (or can contain), except for the subgroups.

This method describing cross-sections in the resonance region was proposed in 1964 by Abagyan et al. [3]. It is at present employed by various reactor-physics groups, especially in the USSR [3] and France [4,5].

In practice, this method can be used to describe the structure of the cross-section (E) in an interval $(E_i E_s)$ by N values of the pair (a_n, σ_n) such that $\Sigma a_n = 1$. The cross section calculations, particularly for self-shielding are made with these N data pairs and the smaller the number N the greater the speed of calculation.

This method is very useful for unresolved resonances.

We believe that it would be advantageous to include the corresponding information in the UKAEA format.

II. PRINCIPAL DIFFERENCES BETWEEN THE TWO FORMATS

1. <u>General Classification Number (see Table 1)</u>

Table 1

General Classification Number (GCN)

GCN - Format URSS	GCN - Format UKAEA
01 - neutron cross-section	01 - neutron cross-section
02 - ang. dist. of secondary particles	02 - ang. dist. of neutrons
03 - en. dist. of secondary particles	03 - en. dist. of neutrons
04 - energy § ang.dist. in thermal neutron scattering	04 - miscellaneous quantities for neutrons
05 - special quantities for neutrons	05, 06 - resonance data for neutron
	07 - thermal neutron scattering law data
	08 to 13 - photons data

The differences appear to be mainly formal: the 04 (UKAEA) becomes 05 (USSR) whilst 07 (UKAEA becomes 04 (USSR).

We would suggest that the USSR format adopt the English code numbers 01-04 and 07, plus the code numbers above 13 for distributions of secondary particles other than neutrons.

2. Particular Classification Number (The differences observed are indicated in Table 2)

The differences seem to be of no practical importance, since they relate to data not at present included in evaluated-data libraries, except perhaps for the reactions 1028, 1029, 1030, 1101, 1107 (UKAEA format).

The USSR format is compatible with the UKAEA format but the inverse is not the case. There seems to be no difference for PCN = 101.

3. Cross-sections (type 1000 data)

The heading cards are shown in Table 3.

Table 2

Particular Classification Number (PCN)

PCN	URSS	PCN	UKAEA
27 to 100	non allocated	27	absorption cross-section = $\sigma_f + \sigma_t$
		28	n, n'p
		29	n, n' 2α
		30	n, 2n 2α
		31-100	non allocated
101	total absorption (without emission of incident particle)	101	disapearance cross-section (without emission of neutron
109-150	non allocated	109	n, pα
		110	distribution = non elastic-total (n, n')
		111-150	available
201-999	non allocated	201 to 208	allocated to some data whic can be deduced from others ones, eventually taking in ac count the transfer matrices.
		301-450	energy release rate parameter ($\overline{\sigma E}$)
		209 to 300 and 451 to 999	non allocated

TABLE III

Comparison of the heading cards for cross sections

(General Classification Number = 1)

Format UKAEA-						
1st card	reaction type number	number of energy intervals	Q reaction	mode of interpolation		
2nd card	lower energy limit - E_i	upper energy limit - E_s	temperature	number of card for this temperature	number of points for this temperature	number of temperatures
Format URSS-						
1st card	reaction type number	number of energy intervals	Q reaction			
2nd card	lower energy limit - E_i	upper energy limit - E_s	number of cards	number of temperature		
3nd card	temperature	number of "Form type number"	number of cards for this temp.			

In the URSS format, the interpolation mode is defined in the 4th card, which depends on the value of "FTN", the "form type number "

The USSR presentation is more logical than the UKAEA presentation especially as regards the inclusion of several temperatures. It is characterized by a new item of information, namely that defining the data type.

The USSR format provides for five cases for each (E_i, E_s) interval. according to the FTN (form type number). The FTN value is the first data element in the fourth card.

- 1st case. FTN = 101. σ is constant in the (E_i, E_s) interval a single value is given.
- 2nd case. FTN = 111. Several values are given for the pair $(E, \sigma(E))$.
- 3rd case. FTN = 112. Subgroup representation. Several values are given for the pair (a_i, σ_i), such that $\Sigma a_i = 1$.
- 4th case. FTN = 121. Subgroup representation for several values of E; for each value of E several values of the pair (a_i, σ_i) are given, such that $\Sigma a_i = 1$ (for each E).
- 5th case. FTN = 122. Subgroup representation for several values of E; for each subgroup i several values of energy E_j are given, together with the corresponding values of a_{ij} and σ_{ij}.

This representation contains the same information as the preceding one.

The 2nd case is the only one which is compatible in form with the present UKAEA format. The 1st case is not really incompatible: a constant cross-section can always be represented by interpolation between two energies having the same cross-section values*/.

The 3rd and 4th cases represent the novel contribution of this format and they cannot be included directly in the present UKAEA format.

The 5th case is a transposition of the 4th case; we do not regard it as of fundamental importance.

4. Angular distribution (type 2000 data)

The presentation of the heading cards is shown in Table 4.

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*/ There is one difficulty: the UKAEA format requires continuity and does not permit representation of the cross-sections by groups, whereas the USSR format apparently does.

TABLE IV

Comparison of the heading cards for angular distribution

(General Classification number =2)

Format UKAEA - energy range wise case.						
1st card	reaction type number	number of energy intervals	atomic mass	reference system	type of data	blank or definition number of energy range for Legendre polynomial distribution
2nd card	lower energy limit	upper energy limit	number of cards	number of distribution	probability of the first angular dist.	number of angles
Format URSS -						
1st card	reaction type number	number of energy intervals	atomic mass	←	— available —	→
2nd card	lower energy limit	upper energy limit	number of cards	number of groups of distributions	← available —	→
3nd card	identification of secondary particles group	number of form type number for this group	number of cards for this group	←	— available —	→

It is understood that the sum of the partial reactions should be equal to the total cross-section in each subgroup.

The number of subgroups varies from one energy band to another, and the most suitable number is clearly the minimum compatible with satisfactory accuracy of the calculations. This problem has not been considered by fast-reactor physicists in France because the subgroup parameters they employ are not obtained from the distribution laws mentioned above but from self-shielding factors calculated in advance.

The USSR format provides for giving the angular distributions in the form of a probability distribution $f(\cos\theta)$ or of Legendre polynomial coefficients w_ℓ, whilst the UKAEA format provides, in addition, for giving differential cross-sections; this does not mean there is any incompatibility (for the translation UKAEA → USSR it is only necessary to renormalize).

However, the presentation of the data is quite different in the USSR format, which distinguishes six cases: for each of these six cases the FTN value 1XX corresponds to a distribution defined by $f(\cos\theta)$ whilst FTN = 2XX relates to a distribution defined by the Legendre polynomial coefficients w_ℓ. In each case the reference system is indicated (laboratory or centre of mass).

The six cases are as follows:

- 1st case. FTN = 101 or 201. Isotropic angular distribution.
- 2nd case. FTN = 102 or 202. A single angular distribution in the interval (E_i, E_s).
- 3rd case. FTN = 111 or 211. Angular distributions for N values of E between E_i and E_s.
- 4th case. FTN = 112 or 212. Addition of several angular distributions in the interval (E_i, E_s) with a weight a_i for each distribution.
- 5th case. FTN = 121 or 221. Addition of several angular distributions for N values of E between E_i and E_s with a weight a_i for each distribution; the number of values of $f(\cos\theta)$ or of w_n is given for each energy and each weight.
- 6th case. FTN = 122 or 222. Addition of several angular distributions for M weights a_i with an energy E for each distribution; the number of values of $f(\cos\theta)$ or w is given for each weight and each energy.

This system is rather different in form from the UKAEA system without offering the possibility of additional information: cases 1-5 are all included in the UKAEA format. Only case 6 is not included, but it is merely a transposition of case 5 and the information it contains can always be presented in the form of case 5 and, hence, in the UKAEA format.

It is pointed out (page 32, or page 19 of the English translation) that the system can be used (for the same RTN) to combine distributions given in different systems, or given sometimes by f(cos θ) and sometimes by w_{ℓ}. We do not see, however, how this can be done in the present system; moreover, the value of this possibility seems rather academic, and the fact that it is not provided for in the UKAEA format can hardly be regarded as a disadvantage.

In short, we consider that the UKAEA format provides for all the information that can be contained in the USSR format.

5. Energy distribution of secondary particles (type 3000 data)

Table 5 compares the types of law permitted by the two formats.

Table 5

Energy Distribution Laws
Correspondence as between the USSR and UKAEA laws

URSS law number	Corresponding UKAEA law number
1	1
2	2
3	no correspondance
4	7
5	4
6	5
7	6
8	no correspondance, but very similar to law 8 (see text)
no correspondance, but can be included in law 5.	3
no correspondance	9 and 10

Laws 8 (USSR) and 8 (UKAEA) are very similar: in the former case the datum is a probability and in the second case it is a cross-section.

Table 6 compares the headings: these differ somewhat in presentation, the USSR format being again more logical than the UKAEA format.

TABLE VI

Comparison of heading cards for secondary particles (or neutrons) energy distribution

Format UKAEA -						
1st card	reaction type number	number of energy intervals	system	←	available	→
2nd card	lower energy limit - E_i	upper energy limit - E_s	number of cards	number of distribution	probability of this distribution	energy distribution law number
Format URSS -						
1st card	reaction type number	number of energy intervals		←	available	→
2nd card	lower energy E_i	upper energy E_s	number of cards	number of secondary particle groups	← available	→
3nd card	flag identifying a group	number of "form type number"	number of cards for this group	←	available	→

The cases provided for are defined by the Form Type Number.

FTN = 101.	Law 1, identical with UKAEA law 1.
FTN = 102.	Law 2, identical with UKAEA law 2.
FTN = 103.	Law 3.
FTN = 104.	Law 4, identical with UKAEA law 7.
FTN = 105)	(Law 5, identical with UKAEA law 4.
106)	(Law 6, identical with UKAEA law 5.
107)	(Law 7, identical with UKAEA law 6.
FTN = 150.	Combination of laws type 1, 2, 3, 4, 5, 6 and 7.
FTN = 208.	Law 8 (similar to UKAEA law 8).
FTN = 251.	Combination of laws type 1-8 for given E. (Energy of incident neutron)
FTN = 252.	Combination of laws type 1-8 for several values of E.

Most of the laws correspond directly to the English format; the combinations (cases FTN = 150, 251, 252) can also be expressed in the English format by repeating the 2nd card of Table 6 each time.

We think that here, too, the USSR format could come closer to the UKAEA format without any loss of information.

6. Angular distribution of thermal neutron energy

Since we are not experts on these data we have not studied the problem.

7. Special data (η, $\bar{\nu}$, $\tilde{\alpha}$)

The presentation of the data is the same as for the cross-sections; a presentation using the subgroup method is pointless and no such presentation exists. The USSR and UKAEA formats are perfectly compatible.

III. DIFFERENCE IN CARD PUNCHING

According to the Kolessov/Nikolaev document the USSR card is as shown below:

1st line	1st information	Auxiliary information for each line (?)
2nd line	2nd information	
3rd line	3rd information	
....	....	
6th line	6th information	
7th line	1st (service) information	
8th line	2nd (service) information	
	4 blank lines	

or:

1st line	1st information	Service information	UKAEA 1st card
....	....		
6th line	6th information		
7th line	1st information		UKAEA 2nd card
....	....		
12th line	6th information		

One USSR card thus corresponds to two UKAEA cards in the second case.

The UKAEA card is shown below:

1 to 12	13 to 24	25 to 36	37 to 48	49 to 60	61 to 72	73 to 80
1st information	2nd information	3rd information	4th information	5th information	6th information	3 service informations

The amount of information appears to be the same in all three cases: a conversion from one type of presentation to the other would require a special programme, written in machine language, but this should not constitute a major difficulty.

Other problems would arise in the not unlikely case of an exchange of evaluations recorded on magnetic tapes: in particular, there would be the risk of physical incompatibility of the magnetic tapes (USSR tapes have 16 tracks).

Some competent authority (such as the IAEA) could help in this connection.

IV. CONCLUSION

The USSR format probably conforms to local requirements, which we are not familiar with: one of the effects of this is in the mode of card punching. However, this does not seem to be a major obstacle as far as conversion from one format to the other is concerned.

This format also is more logical: profiting from experience gained in regard to other formats, it is coherent and modern, whilst the UKAEA format has been developed progressively and, at every stage, has had to incorporate changes dictated by experience.

With the exception of the cross-sections (type 1000 data), however, it contains no information which the UKAEA format cannot contain. Whilst not familiar with local requirements in the USSR, we should like to express the hope that the USSR format could be patterned as closely as possible on the UKAEA format in order - with some sacrifice in logic - to avoid or to simplify as far as possible the problems of translation in either direction.

We think the type 1000 data (cross-sections) could usefully include data resulting from the subgroup method, but it would apparently be necessary to specify the data for inclusion; in the view of the French reactor physicists, as expounded in the attached Annex, the values of $\sigma_t(i)$ and a_i should be given for each subgroup i, as well as $\bar{\sigma}_x(i)$ for each partial cross-section x. We intend to consider this problem further in collaboration with other users of UKAEA tape. In the Annex we attempt to explain the subgroup method.

In conclusion, it should be borne in mind that these libraries are used by programmes which permit, as input, presentations that are much more restricted than that given for the description of the format.

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Annex

Note on the A. Khairallah subgroup method

The subgroup method is at present used in fast reactor physics in France to deal with self-shielding of narrow resonances of heavy elements, either in a homogeneous environment or in a heterogeneous cell.

For this type of treatment integrals of the following type have to be calculated over a given energy interval:

$$I = \int \sigma_x(E) \; \varphi(E) \, dE$$

For example we may have

$$\varphi(E) \sim \frac{1}{\sigma(E) + \sigma_p}$$

where $\sigma_x(E)$ is the cross-section for the reaction x

$\sigma(E)$ is the total cross-section

σ_p is the dilution cross section.

The flux can generally be written in the form $\varphi(_{\sigma(E)})$, so that:

$$I = \int \sigma_x(E) \; \varphi_{(\sigma(E))} \, dE$$

This integral can be written in the form of a Lesbesgue integral

$$I = \int \bar{\sigma}_{x(\sigma)} \; \varphi_{(\sigma)} \; P_{(\sigma)} \, d\sigma$$

where $P_{(\sigma)}$ is the distribution law for σ over the energy interval in question

$\bar{\sigma}_{x(\sigma)}$ is the mean value of $\sigma_x(E)$ for $\sigma(E) = \sigma$.

Defining an energy integration range U such that:

$$\sigma - \frac{d\sigma}{2} < \sigma(E) < \sigma + \frac{d\sigma}{2}$$

we get:

$$P_{(\sigma)} d\sigma = \int_u dE$$

$$\bar{\sigma}_{x(\sigma)} = \frac{\int_u \sigma_x(E) dE}{\int_u dE}$$

In the subgroup method $P_{(\sigma)}$ is represented by a discrete series of values of σ_k with a weight a_k for each value. The values of $\bar{\sigma}_{x_k}$ for each partial reaction x must also be defined.

If the cross-sections are described by subgroups, it therefore seems desirable to have the following information on the tape, for each isotope and each temperature:

a_k, σ_k, $\bar{\sigma}_{x_k}$ (for all the reactions) for each subgroup.

00413