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LIBRARY OF NEUTRON REACTION CROSS-SECTIONS IN THE ABBN-93 CONSTANT SYSTEM

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LIBRARY OF NEUTRON REACTION CROSS-SECTIONS IN THE ABBN-93 CONSTANT SYSTEM. The library of neutron reaction group cross-sections in the ABBN-93 constant set is described. The format used for data representation, the content and purpose of the sub-libraries and their practical application in the SCALE criticality safety estimation system are discussed.

Individual neutron reaction cross-sections were not determined in the ABBN-64 constant system [1]. In the ABBN-78 constant system [2], group cross-sections of the most important neutron reactions were determined, although their use in practical calculations was limited. This was because the ABBN-78 constant system was not intended to be used, nor indeed has it been used, for calculating the radiation characteristics of irradiated materials, where a knowledge of the reaction cross-sections is highly important. The ABBN-93 constant system [3] had greater applicability from the outset. In particular, the intention was to gradually introduce it, *inter alia*, into calculations of the radiation characteristics of irradiated fuel, reactor designs and technological environments. Consequently, from the beginning it was envisaged that the ABBN-93 constant system contain libraries of all the data required to carry out these calculations: fission product yields, decay characteristics of radionuclides and group neutron reaction cross-sections. Although actually these libraries were all set up, in practical terms their application did not, of course, involve the use of ABBN constants in the traditional areas, namely in calculating neutron and photon fields in reactors and in shielding. Instead of using these ABBN constants in the calculations, appropriate constants were used that had previously been included in the data libraries of programs for calculating isotope kinetics and radiation characteristics: CARE [4], ORIGEN [5] and FISPACT [6]. Recently the situation has begun to change. The Standardized Computer Analyses for Licensing Evaluation of nuclear power facilities system (SCALE) [7] allows for certain data used by the CARE and ORIGEN programs to be replaced with data from the ABBN libraries. This relates primarily to data on neutron cross-sections since it is clear that the cross-sections used to calculate isotope kinetics should not differ (not substantially, at any rate) from those used to calculate neutron fields in a reactor. The initial application of the library of group neutron reaction cross-sections also prompted the appearance of the present publication since it became necessary to record the stage of development that had been reached at this point.

A general-purpose library of reaction cross-sections

The first task when setting up the library of neutron reaction cross-sections was to ensure the completeness of the data. It was decided that the library should contain data on:

(a) All stable nuclides;

(b) All actinides with half-lives of more than one day, ranging from Ac-225 to Es-255;

(c) All fission products with half-lives of more than one day;

(d) All radionuclides with half-lives of more than one day that can be formed as a result of two to three sequential neutron reactions from the nuclides listed in the previous points;

(e) Some of the main, shorter-lived nuclides (for example, Xe-135).

In the case of all the above nuclides (including isomers with a half-life of more than one day) the library had to contain group neutron cross-sections for each reaction where the threshold was lower than the upper boundary of the (-1)th ABBN group (13.98 MeV). As far as possible, the contents of the library had to correspond with the evaluated neutron data files in the FOND-2 library, on which the ABBN-93 constant system was based. If the FOND-2 library contained a data file relating to a particular nuclide and, in addition, that file provided information on a particular reaction, then the library of group reaction cross-sections included cross-sections obtained using that file. In the case of reactions for which the FOND-2 library files contained no information (as a rule, reactions with high thresholds and very low cross-sections), the data were taken from other libraries, in particular from the EAF-3 library [8]. During the initial stage, data for all the nuclides for which there were no files in the FOND-2 library were also taken from this library. The second stage involved establishing a more complete correspondence between the library of group reaction cross-sections and the FOND-2 data. In particular, isomer production cross-sections, which, as a rule, were missing from the FOND-2 library, were obtained from the total reaction cross-sections, calculated from data in this library by means of multiplication by the probabilities of isomer production (or of the ground state) used in EAF-3. Moreover, additional MF=9 and (or) MF=10 files, containing data on the branching ratios that had been used, began to be included in FOND-2. As a rule, missing data on the cross-sections of improbable reactions with high thresholds were also included (with compensation on account of cross-sections of the most probable reactions). In this way, a more complete correspondence was achieved between the cross-sections library and the files library.

The most undesirable disparity lay in the divergence between data on reactions in a natural isotopic mixture of basic reactor materials, in those cases where the FOND library contained data only for the natural mixture. This disparity was gradually eliminated by the introduction into the FOND-2 library of data on all the stable isotopes and by obtaining, on the basis of these data, a file for the natural mixture. This was carried out in the case of the files on iron, chromium, nickel, zirconium and others. Differences have now been eliminated between data in the modified version of the FOND-2 - FOND-2.2 [9] - library and the library of neutron cross-sections for the basic reactor materials.

The contents of the library of group cross-sections are given in Table 1. All data in this library are given in 28-group representation. The data format is the standard for tables of ABBN tables of group constants [3]. Each table contains cross-sections of all reactions for all the relatively long-lived isotopes of the element, determined by the NAM identifier. The tables have the identification numbers MF=9 and MT=0. By way of example, a table is given of the group reaction cross-sections for aluminium isotopes (Table 2).

Rows that begin with an asterisk contain a commentary and are not processed by the computer. The first two rows are standard ABBN table heading rows. The first of these contains: the NAM material designation (in this example, NAM=Al - aluminium); numbers that identify the data type (MF=9 and MT=0 for tables of group neutron reaction cross-sections); and the material parameter which characterizes the data given in the table as a whole. In tables of the type under consideration, this is the atomic number, Z. The second heading row contains: LT - the number of rows in the table of data (in tables of the MF=9, MT=0 type, invariably LT=33); LC - the total number of columns in the table (in this example LC=20); LS - the number of columns in one part of the table (in tables of the type under consideration, invariably LS=8); and the read-out format of the data from the row containing LT columns. In tables of group neutron reaction cross-sections, as a rule, LC > LS, i.e. the table is divided up into a number of parts (in the example under consideration - three). Column one is repeated in every part. The first columns of the second and subsequent parts, are not included in the total number of columns, LC.

The contents of the data in the table are determined by the parameters MF and MT. In tables of the type under consideration, column one contains the ABBN group number (from the 1st to the 26th) whilst the remaining columns contain group cross-sections of the appropriate reactions. Reactions are identified by the data contained in the first five rows of each column (i.e. in the third, fourth, fifth, sixth and seventh rows, allowance being made for the table heading rows). The first of these rows contains the identification number of the isotope on which the reaction occurs. This is in numerical form with the part in front of the decimal point having the structure ZZAAAM. Here, ZZ is the atomic number (in this example - 13), AAA is the mass number (in this example - 026 or 027) and M is the number of the metastable state (M=0 for ground states).

The second heading row of the column contains the identification number of the evaluated data library, on the basis of which the cross-sections given in the column have been derived. In this identifier the figure in front of the decimal point signifies the following:

1. FOND library;
2. ENDF/B library;
3. JENDL library;
4. JEF library;
5. BROND library;
8. ADL library;
9. EAF library;

0. Group cross-sections evaluated directly and do not correspond to any library.

The part of the identifier after the decimal point, provided that it is less than 0.7, refers to the version number: 2.06 signifies ENDF/B-6; 3.32 signifies JENDL-3.2, and so on. If this part exceeds 0.9, it refers to the year in which the data evaluation or re-evaluation took place. For example, 0.95 means that the group cross-sections were evaluated directly in 1995.

The third row contains the reaction identification number. The three lowest-order digits of this number in front of the decimal point have precisely the same meaning as the ENDF/B reaction identifier MT. The highest-order digit (number of thousands) indicates the isomeric state in which the product-nucleus is formed. For example, 1016 represents the (n,2n) reaction which results in the formation of a product-nucleus in the first isomeric state, and 0016 represents the same reaction which results in the formation of a product-nucleus in the ground state. Number 6 refers to an (n,2n) reaction which results in the formation of a product-nucleus in any state. This identifier value is only used in cases where no individual isomer production cross-sections are given.

The fourth row contains the product-nucleus identifier. This information is superfluous since the product-nucleus is clearly determined by the target-nucleus and the reaction type identifiers.

The fifth heading row of the column indicates the reaction energy, Q, and is expressed in MeV.

In the columns, these heading rows are followed by the cross-sections, given in barns, for the energy groups whose numbers are indicated in the first column of each part. Any gaps in these columns mean that in energy terms reactions in these groups are impossible. 0.000000 indicates that the reaction cross-section is less than a microbarn.

One of the library annexes is a tolerably accurate evaluation of the activity of materials and structures that are being dismantled, transported, stored or sent for recycling. The library is sufficiently reliable and provides considerable scope for calculating activation channels. On the basis of this library and in conjunction with the UK FISPACT program, calculations were made of the radiation characteristics of materials irradiated in the core of the BN-350 [10] and BN-600 [11] fast reactors. Similar calculations are being carried out for BR-10 reactor designs [12] that are being decommissioned. Studies have also been carried out of the radioecological properties of sodium, lead-bismuth and lead coolants in fast neutron reactors [13].

Libraries of fission product and actinide cross-sections

As has already been mentioned, the first area in which the library of neutron reaction cross-sections could be applied was in calculating the nuclide composition of spent fuel in the SCALE system. For this, it was necessary to extract from the general library data on cross-sections of the fission products and actinides accumulating in the fuel. During the calculation process, the appropriate data drawn from the libraries of nuclide composition calculation programs, and in particular from the ORIGEN program, had to be substituted with these cross-sections. For fission products the main point is to substitute their radiative capture cross-sections: the (n,p), (n,α) and (n,2n) reactions have a far weaker impact on the nuclide composition of fuel and calculating the difference between the cross-sections of these reactions taken in the ORIGEN library and the more up-to-date data from our library is of secondary importance. As regards actinides, there was a need for calculation of the latest data on fission and radiative capture cross-sections and also on (n,2n) and (n,3n) reaction cross-sections.

To make this task easier, two sub-libraries were set up on the basis of the general library, one for fission products and the other for actinides. Each sub-library was presented in the form of a single ABBN table, the first with the parameters NAM=FP, MF=309 and MT=102 and the second with the parameters NAM=ACT, MF=309 and MT=18. The format of the tables was exactly the same as that described above. The first table contained data on the radiative capture cross-sections of 169 fission products and the second contained data on capture, fission and (n,2n) and (n,3n) reaction cross-sections, as well as data on the value of $\bar{\nu}$ for all 60 actinides, for which cross-section data were available in the general library. These sub-libraries started to be used in calculations of the nuclide composition of fast reactor spent fuel. To enable them to be used in thermal reactor nuclide fuel calculations, account had to be taken of the extent to which the thermal group cross-sections depended on the neutron gas temperature. It was proposed that Westcott g-factor be used to this end. Consequently, for all fission products and actinides, whose cross-section behaviour in the thermal region diverged substantially from 1/v, the Westcott g-factors were calculated and presented in the form of standard ABBN tables with MF=7. Putting this into practice showed that, when calculating the nuclide composition of thermal reactor fuel, it was expedient not to use the 28-group constants of fission products and actinides with Westcott g-factors, but instead to set up 299-group libraries of cross-sections of the required reactions and to use these. The reason for this approach was that the neutron field calculations in the SCALE system are carried out in ABBN 299-grouping, and the multigroup (299-group) neutron spectra in fuel, required for convolution of the cross-sections, are available in the system. Thus, 299-group tables were created of fission product capture cross-sections and cross-sections of the main reactions on actinides, differing only in terms of group number from the aforementioned 28-group tables. The 28-group and 299-group cross-sections were derived from exactly the same evaluated data files.

The data from the 299-group libraries of fission product and actinide cross-sections are used in the SCALE system as follows. Using reactor calculation programs, the 299-group integral neutron fluxes are calculated for all fuel-filled areas for which the change in nuclide composition needs to be calculated. In this calculation, the ABBN-93 299-group constants prepared for the CONSYST program are used. When preparing the constants, the resonance self-shielding (blocking) of the cross-sections is calculated. The microconstants of each nuclide, blocked with respect to the composition of each area, are stored in the CONSYST program's GMF output format and are also accessible to the system after the macroscopic 299-group constants for the reactor calculation have been worked out on their basis. Once the reactor calculation is complete and the integral neutron spectra in the fuel areas have been calculated, the single group cross-sections of all the fission products and actinides are worked out for each area (using the standard method of averaging out the cross-sections across the spectrum). Account is taken of the fact that part of the actinides, and at times also part of the fission products, are included in the irradiated fuel composition and in the relevant blocked microconstants obtained by the CONSYST program. The shielded cross-sections, recorded in the aforementioned GMF file are used for all these materials. Data from the 299-group cross-section libraries are used for the remaining fission products and actinides.

Then the integral neutron fluxes are normalized to the given power of the reactor (or of a specific fuel area). To this end, data are used on the original fuel composition (taken from the job prepared for CONSYST), the capture and fission reaction rates on the nuclides in this composition, as well as data on the energy release during these reactions, which are given in the column header rows of the neutron reaction cross-section table (for convenience sake, these data are collected in separate ABBN tables).

The next stage involves substituting the capture and fission cross-sections (as well as the (n,2n) and (n,3n) reaction cross-sections on actinides), taken from the ORIGEN program libraries, with the cross-sections calculated using the ABBN constants. Then, the program is run and, using the neutron fluxes that have been normalized to the power and the given irradiation time regime, the composition of the irradiated fuel is calculated (and if necessary its radiation characteristics).

The composition obtained is used by the SCALE system to formulate reactor calculation tasks at the next burnup step. In the process, the fission poison capture cross-sections may be made more accurate. The term poison means the build-up of fission products, whose concentrations are not explicitly taken into account in the calculation. At the very least, explicit allowance needs to be made for poison-products in thermal reactor calculation. Usually, explicit allowance is made for several additional products with large yields and capture cross-sections. The remaining fission products are "lumped together" in the fission poison. As the fission poison contains a large number of fission products, the cross-sections, averaged out with respect to fission poison composition, are comparatively weakly dependent on that composition, thus allowing "standard" fission poison constants, calculated when its composition has been determined once and for all, to be included in the ABBN constant system. The SCALE system allows for recalculation of the fission poison cross-section at each step, taking its real composition into account. To this end, the fission product concentrations in the fuel burned during the previous steps and the 299-group capture cross-sections are used. The 299-group fission poison capture cross-sections obtained in the subsequent step replace the fission poison radiative capture cross-sections taken from the standard ABBN tables. The cross-sections for all the remaining fission poison neutron constants (aside from the total cross-section, which is calculated as the sum of the partial cross-sections) are left as before.

The SCALE system's method of calculation, as described here, can also be used in conjunction with the Russian CARE program instead of ORIGEN.

Alongside the libraries of group neutron reaction cross-sections in the ABBN 28-group and 299-group, similar tables were created of WIMS 69-group cross-sections. These tables are actively used in the WIMS-ABBN constant system [14], which differs from the original version of the WIMS-D4 program [15] in that it reviews the entire library of constants based on the FOND-2 file library, expands the list of resonance nuclides and includes a number of other improvements that have increased the program's applicability to calculations for thermal reactors with any type of MOX-fuel.

Table 1

Contents of the ABBN-93 activation library

№	Element	Number of isotopes	Number of reactions	№	Element	Number of isotopes	Number of reactions
1	H	3	4	35	Sn	18	320
2	He	1	3	36	Sb	9	201
3	Li	2	13	37	Te	21	373
4	Be	2	9	38	I	8	151
5	B	5	32	39	Xe	15	231
6	N	2	17	40	Cs	8	149
7	O	3	23	41	Ba	15	236
8	F	1	10	42	La	5	83
9	Ne	3	21	43	Ce	9	129
10	Na	2	18	44	Pr	3	44
11	Mo	3	24	45	Nd	11	157
12	Al	2	18	46	Pm	10	142
13	Si	5	35	47	Sm	11	150
14	P	3	26	48	Eu	15	213
15	S	5	45	49	Gd	15	204
16	C	3	32	50	Tb	10	153
17	Ar	7	69	51	Dy	13	186
18	K	5	53	52	Ho	4	59
19	Ca	9	80	53	Er	10	152
20	Sc	5	58	54	Tm	8	114
21	Ti	7	74	55	Yb	10	127
22	V	4	49	56	Lu	11	167
23	Cr	5	49	57	Hf	12	223
24	Mn	4	44	58	Ta	7	146
25	Fe	7	68	59	W	11	178
26	Co	6	71	60	Re	7	116
27	Ni	11	111	61	Os	11	170
28	Cu	5	49	62	Ir	11	224
29	Zn	7	79	63	Pt	13	226
30	Ga	3	38	64	Au	8	148
31	Ge	8	94	65	Hg	14	216
32	As	7	88	66	Pb	9	116
33	Se	10	118	67	Bi	7	105
34	Br	4	56	68	Po	5	79

Table 2

Neutron cross-sections for Al

```
NAM=Al        BIB= ACT  MF=  9  MT=  0   Z = 13.
              LT =  33  LC= 20  LS=  8  LF = (I4,7E9.0)
      130260.  130260.  130260.  130260.  130260.  130260.  130260.
         9.03     9.03     9.03     9.03     9.03     9.03     9.03
          16.      22.      28.      32.     102.     103.     107.
      130250.  110220.  120250.  120240.  130270.  120260.  110230.
     -11.3630  -9.4456  -6.3037 -11.4090  13.0540   4.7858   2.9675
  -1    .0161    .1042    .3993   8.62-3   3.70-4    .1779    .0763
   0   1.01-3    .0216    .2193   1.42-3   3.79-4    .2218    .0791
   1            2.37-4    .0643            2.03-4    .2499    .0773
   2                                       1.00-4    .2499    .0631
   3                                       3.84-5    .2476    .0368
   4                                       1.19-6    .2438    .0207
   5                                       1.00-5    .2319    .0130
   6                                       1.03-5    .1084   5.62-3
   7                                       1.84-5
   8                                       4.90-5
   9                                       9.29-5
  10                                       1.38-4
  11                                       2.06-4
  12                                       3.04-4
  13                                       4.40-4
  14                                       6.49-4
  15                                       9.57-4
  16                                       1.40-3
  17                                       2.06-3
  18                                       3.02-3
  19                                       4.44-3
  20                                       6.51-3
  21                                       9.56-3
  22                                        .0140
  23                                        .0206
  24                                        .0302
  25                                        .0444
  26                                        .1558
*
      130260.  130260.  130270.  130270.  130270.  130270.    130270
         9.03     9.03     1.97     1.97     1.22     1.22      1.22
         111.    1004.    0016.    1016.      22.      28.      102.
      110250.  130261.  130260.  130261.  110230.  120260.   130280.
      -9.3538  -0.2280 -13.0540 -13.2820 -10.0860  -8.2681    7.7229
  -1    .0271   2.67-3 2.972-2    9.57-4 8.1783-3  .080     2.5958-4
   0    .0187   5.51-3 6.877-5    1.63-6 6.5786-5  .040     2.4232-4
   1   2.61-4   5.72-3                             .0006    2.8115-4
   2            5.69-3                                      3.2790-4
   3            4.50-3                                      4.246- 4
   4            6.12-4                                      5.6921-4
   5                                                        7.0219-4
   6                                                        8.4671-4
   7                                                        1.2228-3
   8                                                        2.2116-3
   9                                                        1.1429-3
  10                                                        4.5385-3
  11                                                          3.04-3
  12                                                        2.8717-2
  13                                                        6.5655-4
  14                                                        8.2197-4
```

Table 2 (cont.)

15	1.1575-3
16	1.7047-3
17	2.5273-3
18	3.7540-3
19	5.5940-3
20	8.3420-3
21	1.2430-2
22	1.8563-2
23	2.7728-2
24	4.1377-2
25	6.1873-2
26	2.3104-1

*

	130270.	130270.	130270.	130270.	130270.
	1.22	9.03	9.03	1.97	1.97
	103.	104.	105.	0107.	1107.
	120270.	120260.	120250.	110240.	110241.
	-1.8260	-6.0441	-10.8780	-3.1293	-3.6013
-1	7.3790-2	.0189	6.13-3	.0815	.0359
0	9.4496-2	6.56-3	3.16-5	.0759	.0346
1	7.9561-2	8.84-5		.0296	.010
2	2.4491-2			.000213	.000135
3	2.413- 3			.000000	.000000
4	1.6391-6				
5					
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