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EVALUATION OF THE ETOG-3Q, ETOG-3, FLANGE-II, XLACS, NJOY AND LINEAR/RECENT/GROUPIE CODES IN RELATION TO RESONANCE CONTRIBUTIONS AND BACKGROUND COLLISION CROSS-SECTIONS

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ABSTRACT

The NJOY and LINEAR/RECENT/GROUPIE calculational procedures for the resolved and unresolved resonance contributions and background collision cross-sections were evaluated. Elastic scattering, fission and capture multigroup cross-sections generated by these codes and the previously validated ETOG-3Q, ETOG-3, FLANGE-II and XLACS are compared. Constant weighting function and zero Kelvin temperature are assumed. Discrepancies are presented and analysed.

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CONTENTS

1. INTRODUCTION

The compilation of multigroup cross-section libraries is of considerable importance for the analysis of reactor cells. The computer programs which generate these libraries on the basis of evaluated nuclear data (FRENDL [1], ENDF/B-IV [2], etc.) must be validated to ensure that the libraries are coherent and reliable. This report covers the first phase of the validation work on the codes used to generate the multigroup cross-sections. The contribution of resonances (resolved and unresolved) and the background cross-sections were analysed with a constant weighting function and at zero degrees Kelvin. Validation of the codes ETOG-3Q [3], ETOG-3 [4] and FLANGE-II [5] is dealt with in Ref. [3] and that of the code XLACS [6, 7] in Ref. [8]. The final corrected versions of the validated codes are reproduced and the remaining discrepancies are summarized. The results of LINEAR/RECENT/GROUPIE [9-11] and NJOY [12] are included in the evaluation.

Section 2 contains general considerations and Sections 3 to 8 deal with the evaluation of codes ETOG-3Q, ETOG-3, FLANGE-II, XLACS, LINEAR/RECENT/GROUPIE and NJOY respectively. Conclusions and recommendations appear in section 9.

2. GENERAL CONSIDERATIONS

The materials processed are listed in Appendix A. The first five materials were taken from FRENDL [1] library and the rest from ENDF/B-IV [2].

These materials were separated into a compact library generated by the MERGER [13] programme which selected, from the FRENDL and ENDF/B-IV, for each material, archives 1 (General information), 2 (Resonance parameters), and from archive 3 (Background cross-sections) the elastic scattering, fission and capture reactions. This procedure optimizes the computation time and was used for all the codes, except NJOY. For NJOY the complete materials were separated, because the code uses information from the dictionary (MF = 1, MT = 451) of the library of evaluated nuclear data which MERGER does not update when generating the compact library.

The epithermal (MUFT) and thermal (THERMOS) energy structures [14] used for ETOG-3 and FLANGE-II respectively are given in Appendix B. In order to check the consistency of the cross-sections in the interface group between the ETOG-3 and FLANGE-II codes the 54 group limits of the MUFT structure were replaced by the 30 Group 30 limits of the THERMOS structure. The resulting structure, composed of 83 groups, was adopted for XLACS, NJOY and GROUPIE.

Some of the principal discrepancies in the multigroup cross-sections generated are given in the form of tables, by reaction and material. See Appendix C, obtained as an auxiliary of the COMPAR system [15, 16].

3. ETOG-3Q CODE

ETOG-3Q, a result of applying Gaussian quadratures to the reconstruction and integration of resolved resonances in ETOG-3, produces multigroup cross-sections of proven precision [3]. This code, with 32 quadrature points, was considered as a reference in the entire energy structure used. The one inconsistency which still persists lies in the interpretation of parameters in the unresolved resonance region. Interpolation in the cross-sections was tried here; however, according to Cullen [17] and also according to the recommendation of ENDF/B, interpolation for ENDF/B-IV should be in the parameters and not in the cross-sections.

Discrepancies were observed between the two procedures in the cross-sections for ^{235}U, ^{239}Pu and ^{241}Pu. Appendix C shows as an example the capture cross-section of ^{241}Pu, for which the correct values are those of CULLEN-87 (defined in Section 7).

4. ETOG-3 CODE

There remain, in ETOG-3, apart from the matter of unresolved resonances broached in the previous section, two discrepancies which are summarized in Ref. [3].

Elastic scattering

The number of points is insufficient for reconstructing all the resonances if there are many resonances in the group.

This fact was observed in the cross-sections for ^{177}Hf, ^{179}Hf, Ni, Cr, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{232}Th - Appendix C shows the relevant results for ^{179}Hf and ^{238}U.

Capture and fission

The "1/v tail" treatment used for the code entails discrepancies which can be observed in the resolved resonance region for all the materials. The materials ^{241}Am and ^{241}Pu are listed as examples in Appendix C.

5. FLANGE-II CODE

This shows no deviation of more than 0.05% compared to Ref. [3].

6. XLACS CODE

This shows no deviation of more than 0.15% compared to Ref. [8]; however, the unresolved resonance region is incorrectly interpreted, as discussed in Section 3.

7. LINEAR/RECENT/GROUPIE CODES

Two versions of these codes were evaluated. The one defined as CULLEN-84 corresponds to versions 84-1 of the group of codes, and that defined as CULLEN-87 corresponds to LINEAR and RECENT 87-1 and to GROUPIE 86-1. The tolerance used in the linearization and reconstruction was 0.5%.

The evaluation of the two versions produced the following observations.

(a) States not permitted in the resolved resonance region are described by the multi-level Breit-Wigner formalism.

CULLEN-84 does not accept such states. The material is not processed - instead a message is printed specifying the problem.

CULLEN-87 processes the materials and prints a message alerting readers to the problem.

This situation arose with ^{177}Hf and ^{179}Hf; the latter is included in Appendix C.

(b) An incorrect interpretation by CULLEN-84 of the parameters in the unresolved resonance region (URR) for ^{241}Am from ENDF/B-IV.

For this material, the parameters LFW-1 and LRF-1, which signify "average fission width" and "only average fission widths are energy-dependent", respectively, are provided for the URR. If there are fission widths, the parameters should be supplied; however, for this material, in the ENDF/B-IV, they are void.

CULLEN-84 incorrectly interprets the parameters with resulting errors in scattering and capture. This was confirmed by the following test. LFW was changed from 1 to 0 and the remaining parameters of archive 2 were altered correspondingly. The discrepancies disappeared, which confirms the error in interpretation of the parameters.

CULLEN-87 provides correct results. See Appendix C.

(c) Resonance region: parameter, versus cross-section interpolation.

CULLEN-84 interpolates in the cross-sections and CULLEN-87 the parameters (see comments in Section 3). At present, we do not have any means of evaluating the procedure adopted by CULLEN-87 and recommended for ENDF/B.

(d) In general, in terms of deviations, CULLEN-87 provides better results than CULLEN-84.

8. NJOY CODE

The version of the NJOY code which we have available is from 1983. The tolerance used in the reconstruction was 0.5%.

Evaluation of the results obtained leads to the following observations.

(a) States not permitted in the resolved resonances of the multi-level Breit-Wigner formalism.

These states are disregarded, but no advice or instruction is given. This occurs with ^{177}Hf and ^{179}Hf and is seen in Appendix C for ^{179}Hf. Confirmation of this was obtained by processing ETOG-3Q without the resonances which were the source of the problem.

(b) Incorrect interpretation of the "background" for ^{241}Am in ENDF/B-IV. The fission contribution in the URR, stems solely from the background, archive 3. However, there is a wide oscillation of background in this region and the code interprets this as being void (see results in Appendix C).

(c) Negative point collision cross-sections for elastic scattering are zeroed.

The discrepancies involved in this procedure were observed in ^{149}Sm, Ni, Cr, ^{238}U and Zirc-2 (represented by Cr and ^{238}U in Appendix C). This was confirmed by running the procedure in CULLEN-84, which produced the same discrepancies. If the card

which implements this process in NJOY is withdrawn, that is if negative point cross-sections are permitted, the execution of NJOY is interrupted by processing error.

(d) Interpolation in the cross-sections, instead of in the parameters, in the unresolved resonances region (see Section 3).

9. CONCLUSIONS AND RECOMMENDATIONS

A system was developed for evaluating the ETOG-3Q, ETOG-3, FLANGE-II, XLACS, NJOY and LINEAR/RECENT/GROUPIE code group which can be extended to other codes which generate multigroup collision cross-sections.

The codes were evaluated, in relation to the contribution of resonances and background cross-sections, for constant weighting function and zero degrees Kelvin. Residual discrepancies are considered in the light of user requirements and with a view to appropriate corrections being made by those who prepared the codes.

Our recommendations are:

- To make full use of the experience acquired in this work to develop an efficient and fast code for multigroup cross-sections, which can be implemented in PC-type computers;

- To follow up the evaluation of the codes by giving attention to weighting functions, temperature effects and transfer matrices (archives 4 and 5 of ENDF/B); and

- To study the influence of corrections in the cross-sections at cell level.

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APPENDIX A

Materials Processed

Material	Identification
72-Hf-176	440
72-Hf-177	441
72-Hf-178	442
72-Hf-179	443
72-Hf-180	444
62-Sm-149	1027
64-Gd-nat	1030
92-U -234	1043
95-Am-241	1056
95-Am-243	1057
47-Ag-107	1138
47-Ag-109	1139
94-Pu-242	1161
92-U -236	1163
28-Ni-nat	1190
24-Cr-nat	1191
26-Fe-nat	1192
25-Mn- 55	1197
92-U -233	1260
92-U -235	1261
92-U -238	1262
94-Pu-239	1264
94-Pu-240	1265
94-Pu-241	1266
Zirc-2	1284
42-Mo-nat	1287
90-Th-232	1296

The first five materials were obtained from the FRENDL [1] library; the rest from ENDF/B–IV [2].

APPENDIX B

Energy Structure Used

B.1 Epithermal structure - MUFT (modified group 54)

MULTIGROUP STRUCTURE

GROUP	ENERGY RANGE	LETHARGY RANGE	GROUP	ENERGY RANGE	LETHARGY RANGE
1	7.7880E+06 - 1.0000E+07	0.000 - .250	28	1.2341E+03 - 2.0347E+03	8.500 - 9.000
2	6.0653E+06 - 7.7880E+06	.250 - .500	29	7.4852E+02 - 1.2341E+03	9.000 - 9.500
3	4.7237E+06 - 6.0653E+06	.500 - .750	30	4.5400E+02 - 7.4852E+02	9.500 - 10.000
4	3.6788E+06 - 4.7237E+06	.750 - 1.000	31	2.7536E+02 - 4.5400E+02	10.000 - 10.500
5	2.8650E+06 - 3.6788E+06	1.000 - 1.250	32	1.6702E+02 - 2.7536E+02	10.500 - 11.000
6	2.2313E+06 - 2.8650E+06	1.250 - 1.500	33	1.3007E+02 - 1.6702E+02	11.000 - 11.250
7	1.7377E+06 - 2.2313E+06	1.500 - 1.750	34	1.0130E+02 - 1.3007E+02	11.250 - 11.500
8	1.3534E+06 - 1.7377E+06	1.750 - 2.000	35	7.8893E+01 - 1.0130E+02	11.500 - 11.750
9	1.0540E+06 - 1.3534E+06	2.000 - 2.250	36	6.1442E+01 - 7.8893E+01	11.750 - 12.000
10	8.2085E+05 - 1.0540E+06	2.250 - 2.500	37	4.7851E+01 - 6.1442E+01	12.000 - 12.250
11	6.3926E+05 - 8.2085E+05	2.500 - 2.750	38	3.7267E+01 - 4.7851E+01	12.250 - 12.500
12	4.9787E+05 - 6.3926E+05	2.750 - 3.000	39	2.9023E+01 - 3.7267E+01	12.500 - 12.750
13	3.8774E+05 - 4.9787E+05	3.000 - 3.250	40	2.2603E+01 - 2.9023E+01	12.750 - 13.000
14	3.0197E+05 - 3.8774E+05	3.250 - 3.500	41	1.7603E+01 - 2.2603E+01	13.000 - 13.250
15	2.3518E+05 - 3.0197E+05	3.500 - 3.750	42	1.3710E+01 - 1.7603E+01	13.250 - 13.500
16	1.8316E+05 - 2.3518E+05	3.750 - 4.000	43	1.0677E+01 - 1.3710E+01	13.500 - 13.750
17	1.4264E+05 - 1.8316E+05	4.000 - 4.250	44	8.3153E+00 - 1.0677E+01	13.750 - 14.000
18	1.1109E+05 - 1.4264E+05	4.250 - 4.500	45	6.4760E+00 - 8.3153E+00	14.000 - 14.250
19	8.6517E+04 - 1.1109E+05	4.500 - 4.750	46	5.0435E+00 - 6.4760E+00	14.250 - 14.500
20	6.7379E+04 - 8.6517E+04	4.750 - 5.000	47	3.9279E+00 - 5.0435E+00	14.500 - 14.750
21	4.0868E+04 - 6.7379E+04	5.000 - 5.500	48	3.0590E+00 - 3.9279E+00	14.750 - 15.000
22	2.4788E+04 - 4.0868E+04	5.500 - 6.000	49	2.3824E+00 - 3.0590E+00	15.000 - 15.250
23	1.5034E+04 - 2.4788E+04	6.000 - 6.500	50	1.8554E+00 - 2.3824E+00	15.250 - 15.500
24	9.1188E+03 - 1.5034E+04	6.500 - 7.000	51	1.4395E+00 - 1.8554E+00	15.500 - 15.754
25	5.5308E+03 - 9.1188E+03	7.000 - 7.500	52	1.1254E+00 - 1.4395E+00	15.754 - 16.000
26	3.3546E+03 - 5.5308E+03	7.500 - 8.000	53	7.8493E-01 - 1.1254E+00	16.000 - 16.360
27	2.0347E+03 - 3.3546E+03	8.000 - 8.500	54	6.2481E-01 - 7.8493E-01	16.360 - 16.588

B.2 Thermal structure – THERMOS

GROUP	ENERGY	VELOCITY	WEIGHT	E BOUNDARY	V BOUNDARY
				.0000633	.0500000
1	.0002530	.1000000	.0005060	.0005693	.1500000
2	.0010120	.2000000	.0010120	.0015813	.2500000
3	.0022770	.3000000	.0015180	.0030993	.3500000
4	.0040480	.4000000	.0020240	.0051233	.4500000
5	.0063250	.5000000	.0025300	.0076533	.5500000
6	.0091080	.6000000	.0030360	.0106893	.6500000
7	.0123970	.7000000	.0035420	.0142313	.7500000
8	.0161920	.8000000	.0040480	.0182793	.8500000
9	.0204930	.9000000	.0045540	.0228333	.9500000
10	.0253000	1.0000000	.0050600	.0278933	1.0500000
11	.0306130	1.1000000	.0055660	.0334593	1.1500000
12	.0364320	1.2000000	.0060720	.0395313	1.2500000
13	.0427570	1.3000000	.0065780	.0461093	1.3500000
14	.0495880	1.4000000	.0070840	.0531933	1.4500000
15	.0569250	1.5000000	.0075900	.0607833	1.5500000
16	.0651734	1.6050000	.0089334	.0697167	1.6600000
17	.0748475	1.7200000	.0104438	.0801605	1.7800000
18	.0861218	1.8450000	.0121364	.0922969	1.9100000
19	.0991861	1.9800000	.0140263	.1063233	2.0500000
20	.1139767	2.1225000	.0155728	.1218960	2.1950000
21	.1312313	2.2775000	.0190148	.1409109	2.3600000
22	.1524837	2.4550000	.0236024	.1645133	2.5500000
23	.1790127	2.6600000	.0296111	.1941244	2.7700000
24	.2124063	2.8975000	.0373864	.2315108	3.0250000
25	.2546383	3.1725000	.0473559	.2788667	3.3200000
26	.3081565	3.4900000	.0600420	.3389087	3.6600000
27	.3759839	3.8550000	.0760746	.4149833	4.0500000
28	.4618327	4.2725000	.0962039	.5111871	4.4950000
29	.5665730	4.7322500	.1136199	.6248070	4.9695000
30	.7025877	5.2697500	.1601229	.7849300	5.5700000

APPENDIX C

Examples of the principal discrepancies encountered in the multigroup cross-sections generated

The following explanations and definitions will help in understanding the results presented in the tables, belonging to this appendix.

- The tables were obtained with the help of a modified version of the COMPAR program [16]. The program was altered to permit inclusion of the three symbols R↓, R↑, U↑, which are indicators of the lower and upper limits of the resolved resonance region, and of the upper limit for the unresolved resonance region.

- The numbers of the groups are given in both increasing and decreasing order of energy.

- The following are presented: multigroup data, percentage deviations in relation to the background, mean square deviation (RMS) and weighted mean square deviation for the background cross-section (RMSP).