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DEVELOPMENT OF INDIAN CROSS SECTION DATA FILES FOR Th-232 AND U-233 AND INTEGRAL VALIDATION STUDIES

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Abstract: This paper presents an overview of the tasks performed towards the development of Indian cross section data files for Th-232 and U-233. Discrepancies in various neutron induced reaction cross sections in various available evaluated data files have been obtained by processing the basic data into mutigroup form and intercomparison of the latter. Interesting results of integral validation studies for capture, fission and (n,2n) cross sections for Th-232 by analyses of selected integral measurements are presented. In the resonance range, energy regions where significant differences in the calculated self-shielding factors for Th-232 occur have been identified by a comparison of self-shielded multigroup cross sections derived from two recent evaluated data files, viz., ENDF/B-V (Rev.2) and JENDL-2, for several dilutions and temperatures. For U-233, the three different basic data files ENDF/B-IV, JENDL-2 and ENDL-84 were intercompared. Interesting observations on the predictional capability of these files for the criticality of the spherical metal U-233 system are given. The current status of Indian data file is presented.

(Th-232, U-233, evaluation, integral testing, nuclear data, optical-statistical model calculations, critical experiments, self shielding factors, data processing, comparisons)

I. Introduction

Thorium is acknowledged /1-3/ as the nuclear fuel in the coming century in the Indian nuclear power programme. It is desirable /4/ to improve the quality of neutron interaction cross section data for Th-232 and U-233 mainly from following three considerations. a. Experimental studies on thorium based reactor systems are to be interpreted on a sound scientific basis. b. Meaningful conceptual design studies involving thorium in different environments such as advanced fast breeders/reactors, fission-fusion hybrids etc. are to be performed and reliable assessments and conclusions are to be drawn. c. Neutron-interaction cross section data base should have finer details and better qualilty in order to aid our basic knowledge of the nuclear structure and to lead to improved studies on nuclear models.

This paper gives an overview of the tasks performed and interesting results obtained/4-16/ within the scope of IGCAR-IAEA Co-ordinated Research Programme on Validation and Benchmark Testing of Actinide Nuclear Data. The programme of work within the scope of this Research Contract (No.3690/R2/RB) is directed towards integral validation of neutron cross sections and development of best cross section data files for Th-232 and U-233.

II. The development of Indian cross section data file in ENDF/B format for Th-232 and U-233

The development of Indian cross section data file in ENDF/B format and subsequent integral validation studies for Th-232 and U-233 is being continued by the Kalpakkam team starting from the evaluations performed in Trombay by M. K. Mehta and his co-workers / 17-24, 26/. These covered evaluations of σ_t , σ_e , σ_{in} , $\sigma_{n,xn}$, σ_f , σ_γ , and $\bar{\nu}$ in the energy region 150 keV to 20 MeV for Th-232. A re-evaluation of capture cross section was reported by Jain and Kailas /24/ using FISPRO /25/ code in 0.1 to 1.2 MeV energy region. The Kalpakkam calculations /13/ made use of late Prof. Peter Moldauer's ABAREX code including width fluctuation corrections for all the neutron cross sections in 10 keV to 4 MeV energy region.

The EXFOR data received from IAEA upto Feb. 1988 is being used in the current evaluations.

For U-233, the evaluation /15/ of resolved and unresolved resonance parameters was carried out and further updating using recent EXFOR data is in progress. The neutron data evaluations carried out on U-233 in Trombay /23/ and in Kalpakkam /15/ thus far are still in a preliminary stage. Using multigroup constants obtained by our processing three available evaluated data files viz. ENDF/B-IV/27/, JENDL-2 /28-29/ and ENDL-84 /30/, the integral validation studies in the fission source energy range by analyses of U-233 spherical JEZEBEL Assembly /31/ and the analyses of U-233 irradiation experiment /32/ in RAPSODIE experimental fast Reactor have been performed.

For the integral validation studies of Th-232 cross sections, initially seven different files were processed and intercompared. These files are: ENDF/B-IV/27/, JENDL-1/33/,Rumanian file/34/, JENDL-2/28-29/, ENDF/B-V(Rev.2)/35/, ENDL-84,/30/and INDIAN file/4-9/.

The neutron interaction cross section data for INDIAN file for Th-232 in ENDF/B format was created on a magnetic tape as per following specification and the tape was transmitted to Dr. Lemmel, Project Officer for this research contract for suggestions and feedback. A.Capture cross section for 50 keV to 20 MeV has been taken from Trombay /19/ evaluation. B.The use of Meadows /36/ fission cross section upto 20 MeV from threshold. C. The (n,2n) cross sections were accepted as in JENDL-2 file based on our results of integral validation studies. In order to have a complete file in ENDF/B format these partial data recommended by us were put in ENDF/B-IV format by starting with JENDL-2 File. Further updating is expected to be made in the future.

III. Proccesing of basic evaluated data files and intercomparison of multigroup constants for Th-232 and U-233

The extensive new comparisons of infinite dilution cross sections, self-shielded cross sections and their Doppler changes for Th-232 calculated by processing recent data files JENDL-2 and ENDF/B-V (Rev. 2) have been completed and results have revealed/8-9/ large discrepancies.

The resonance parameters in various data files for Th-232 do not agree with each other. The differences in resonance characteristics in two evaluated neutron cross section data files reflect as differences in infinite dilution cross sections and the associated self-shielding

Table 1 Comparison of self-shielded cross sections for capture in Th-232

Group no:16; Energy region: 2040.0 eV to 3360.0 eV

	JENDL-2	ENDF/B-V	DIFF*
IDCCS(barns) :	1.180	1.640	38.983

	Temperature :300.0 Kelvin			Temperature :2100.0 Kelvin			DOPPLER CHANGE FOR 300 to 2100K		
SIGO (barns)	JENDL-2 SSCS	ENDF/B-V SSCS	DIFF	JENDL-2 SSCS	ENDF/B-V SSCS	DIFF	JENDL-2 ΔSSCS	ENDF/B-V Δ SSCS	DIFFDC
0.	0.49711	0.82902	66.768	0.74739	1.12466	50.479	0.25028	0.29564	18.126
10.0	0.61752	0.96811	56.774	0.85531	1.24796	45.907	0.23779	0.27985	17.686
100.0	0.92348	1.32455	43.430	1.06740	1.49904	40.438	0.14392	0.17450	21.241
1000.0	1.13494	1.58290	39.470	1.16416	1.61970	39.130	0.02923	0.03680	25.910
10000.0	1.17506	1.63369	39.031	1.17835	1.63787	38.997	0.00329	0.00418	27.028
100000.0	1.17950	1.63936	38.987	1.17983	1.63979	38.984	0.00033	0.00043	29.058

Table 2 Comparison of infinite dilution cross sections, self shielded cross sections and Doppler changes in self shielded cross sections at a dilution of 100 barns for Th-232.

GROUP	LOWER ENERGY (eV)	UPPER ENERGY (eV)	R/UR	DIFF*	DIFF AT 300K	DIFF AT 2100K	DIFFDC
10	40930.000	67480.000	UR	7.246	7.246	6.185	-100.000
11	24830.000	40930.000	UR	-4.086	-3.990	-4.086	- 23.269
12	15600.000	24830.000	UR	-4.530	-4.433	-4.530	- 13.209
13	9130.000	15600.000	UR	-3.960	-3.666	-3.864	- 14.070
14	5540.000	9130.000	UR	-3.759	-3.457	-3.564	- 6.967
15	3360.000	5540.000	UR	2.913	4.803	4.134	- 6.276
16	2040.000	3360.000	R	38.983	43.430	40.438	21.241
17	1240.000	2040.000	R	15.306	18.235	16.145	7.689
18	749.680	1240.000	R	22.283	24.666	23.177	16.771
19	454.710	749.680	R	22.652	17.988	17.751	17.137
20	275.790	454.710	R	9.136	12.494	10.663	7.415
21	101.460	275.790	R	2.362	10.198	7.889	4.406
22	22.640	101.460	R	1.395	2.896	1.695	- 0.738
23	3.060	22.640	R	9.375	12.805	7.810	0.126
24	0.414	3.060	R	25.933	25.994	25.992	- 37.029
25	thermal		R	2.213	2.210	2.212	- 18.228

Note:

R: Resolved Resonance Region; UR: Unresolved Resonance Region

IDCCS = Infinite Dilution Capture Cross Section (barns)

DIFF* = Percentage difference in the infinite dilution capture cross section
= {[IDCCS(ENDF/B-V) - IDCCS(JENDL-2)]/ IDCCS(JENDL-2)}*100.

SSCS :Self Shielded Cross Section (barns) at a dilution of 100 barns at the given temperature.

DIFF : Percentage difference in the self shielded cross section at a dilution of 100 barns at the given temperature.
= {[SSCS(ENDF/B-V) -SSCS(JENDL-2)] / SSCS(JENDL-2)}*100.

Δ SSCS : Doppler change in the self shielded cross section (barns) at a dilution of 100 barns for the change of temperature from 300K to 2100K.
= SSCS(2100K) - SSCS(300K)

DIFFDC = Percentage difference in Doppler change in the self shielded cross section at a dilution of 100 barns for the change of temperature from 300K to 2100K.
= {[ΔSSCS(ENDF/B-V) - Δ SSCS(JENDL-2)] / Δ SSCS(JENDL-2)}* 100.

Table 3 Comparison of multigroup capture cross sections for U-233

GROUP	UPPER ENERGY	JENDL-2 (BARNS)	RATIO ENDL / JENDL-2	RATIO ENDF/BIV / JENDL-2	RATIO FRENCH / JENDL-2	MEAN DEVIATION (IN PERCENT)			
						JENDL-2	ENDL	ENDF/BIV	FRENCH
1	14.5 MeV	0.3870E-02	2.1395	4.4961	2.2997	-36.30	36.30	186.40	46.50
2	3.68 MeV	0.3030E-01	0.5941	0.8878	0.6007	25.47	-25.47	11.39	-24.64
3	2.23 MeV	0.8380E-01	0.3890	0.4630	0.4212	43.99	-43.99	-33.33	-39.35
4	1.36 MeV	0.1130E 00	0.5920	0.4867	0.7080	25.63	-25.63	-38.85	-11.06
5	822.0 KeV	0.1220E 00	0.9426	0.8361	1.0246	2.95	-2.95	-13.92	5.49
6	499.0 KeV	0.1460E 00	1.1849	1.1027	1.1781	-8.46	8.46	0.94	7.84
7	302.0 KeV	0.1830E 00	1.1803	1.0820	1.1257	-8.27	8.27	-0.75	3.26
8	183.0 KeV	0.2320E 00	0.9612	0.9138	1.0086	1.98	-1.98	-6.81	2.86
9	111.0 KeV	0.2610E 00	0.8851	0.8851	1.0421	6.10	-6.10	-6.10	10.57
10	67.5 KeV	0.2740E 00	1.0000	1.0000	1.0438	0.	0.	0.	4.38
11	40.9 KeV	0.2850E 00	1.1579	1.1579	1.2561	-7.32	7.32	7.32	16.42
12	24.8 KeV	0.2900E 00	1.3586	1.3586	1.6552	-15.20	15.20	15.20	40.35
13	15.1 KeV	0.3360E 00	1.4018	1.4018	1.8750	-16.73	16.73	16.73	56.13
14	9.13 KeV	0.4290E 00	1.3287	1.3263	3.0070	-14.11	14.11	13.91	158.30
15	5.54 KeV	0.6040E 00	1.1424	1.1407	2.5000	-6.65	6.65	6.49	133.40
16	3.36 KeV	0.8350E 00	1.0084	1.0072	2.0719	-0.42	0.42	0.30	106.30
17	2.04 KeV	0.9150E 00	0.9814	0.9803	2.2186	0.94	-0.94	-1.05	123.90
18	1.24 KeV	0.1320E 01	0.8333	0.8333	2.0455	9.09	-9.09	-9.09	123.10
19	750.0 eV	0.1760E 01	0.8864	0.8864	1.6477	6.02	-6.02	-6.02	74.70
20	455.0 eV	0.1500E 01	1.4933	1.4933	4.4667	-19.79	19.79	19.79	258.30
21	276.0 eV	0.3310E 01	1.0665	1.0665	3.2931	-3.22	3.22	3.22	218.70
22	101.0 eV	0.5050E 01	1.0277	1.0297	2.9703	-1.37	1.37	1.56	193.00
23	22.6 eV	0.1790E 02	1.0335	1.0279	1.7318	-1.65	1.65	1.10	70.33
24	3.06 eV	0.6620E 02	0.9894	0.9849	1.1329	0.53	-0.53	-0.99	13.90
25	0.414 eV	0.4530E 02	1.0155	1.0132	1.0728	-0.77	0.77	0.55	6.46

Table 4 Comparison of multigroup fission cross sections for U-233

GROUP	UPPER ENERGY	JENDL-2 (BARNS)	RATIO ENDL / JENDL-2	RATIO ENDF/BIV / JENDL-2	RATIO FRENCH / JENDL-2	MEAN DEVIATION (IN PERCENT)			
						JENDL-2	ENDL	ENDF/BIV	FRENCH
1	14.5 MeV	0.1680E 01	1.0179	0.9702	1.0298	-0.88	0.88	-3.84	2.06
2	3.68 MeV	0.1820E 01	1.0000	0.9780	1.0659	0.	0.	-2.20	6.59
3	2.23 MeV	0.1930E 01	0.9896	0.9741	1.0363	0.52	-0.52	-2.08	4.17
4	1.36 MeV	0.1870E 01	1.0053	0.9786	1.0481	-0.27	0.27	-2.40	4.53
5	822.0 KeV	0.1920E 01	1.0104	0.9375	1.0521	-0.52	0.52	-6.74	4.66
6	499.0 KeV	0.2050E 01	1.0341	0.9756	1.0488	-1.68	1.68	-4.08	3.12
7	302.0 KeV	0.2190E 01	1.0137	0.9817	1.0274	-0.68	0.68	-2.49	2.04
8	183.0 KeV	0.2170E 01	1.0369	1.0046	1.0599	-1.81	1.81	-1.36	4.07
9	111.0 KeV	0.2290E 01	1.0349	0.9869	1.1135	-1.72	1.72	-3.00	9.44
10	67.5 KeV	0.2470E 01	1.0688	1.0324	1.0526	-3.33	3.33	-0.20	1.76
11	40.9 KeV	0.2730E 01	1.0806	1.0842	1.1722	-3.87	3.87	4.23	12.68
12	24.8 KeV	0.3120E 01	1.1090	1.0994	1.1859	-5.17	5.17	4.25	12.46
13	15.1 KeV	0.3690E 01	1.1138	1.0921	1.1382	-5.38	5.38	3.33	7.69
14	9.13 KeV	0.4440E 01	1.1081	1.0833	1.5315	-5.13	5.13	2.78	45.30
15	5.54 KeV	0.5260E 01	1.1369	1.0989	1.3688	-6.41	6.41	2.85	28.11
16	3.36 KeV	0.6830E 01	1.0878	1.0264	1.1567	-4.21	4.21	-1.68	10.80
17	2.04 KeV	0.8530E 01	1.0750	1.0680	0.9906	-3.62	3.62	2.94	-4.52
18	1.24 KeV	0.1090E 02	1.0183	1.0183	0.8899	-0.91	0.91	0.91	-11.82
19	750.0 eV	0.1320E 02	1.0152	1.0152	0.9470	-0.75	0.75	0.75	-6.01
20	455.0 eV	0.1580E 02	1.0570	1.0570	1.0127	-2.77	2.77	2.77	-1.54
21	276.0 eV	0.2310E 02	1.0043	1.0043	1.0823	-0.22	0.22	0.22	7.99
22	101.0 eV	0.4150E 02	0.9542	0.9518	1.1325	2.34	-2.34	-2.59	15.91
23	22.6 eV	0.1160E 03	0.9741	0.9828	0.9483	1.31	-1.31	-0.44	-3.93
24	3.06 eV	0.2400E 03	0.9750	0.9875	0.9375	1.27	-1.27	0.	-5.06
25	0.414 eV	0.5300E 03	0.9943	0.9906	0.9896	0.28	-0.28	-0.66	-0.76

Note: Mean deviation for the multigroup cross section of a given file is defined here as the deviation of the multigroup cross section of a given file from the mean value. In the calculation of the mean value of multigroup cross section only the two recent files, viz. JENDL-2 and ENDL-84 files are considered.

The resonance parameters in various data files for Th-232 do not agree with each other. The differences in resonance characteristics in two evaluated neutron cross section data files reflect as differences in infinite dilution cross sections and the associated self-shielding effects. The data in the two evaluated basic data files may be considered to represent mean values of two populations (or samples) of the ensemble. If the group constants of two data files for a given temperature and background dilution agree with each other, that is, there is no discrepancy, it does not necessarily mean that there is no error in the data. A systematic error may still exist and the effective group constants of two data files may differ from the true values. A comparison is nevertheless certainly helpful to identify possible problem areas in the resonance region.

In order to make sure that processing of basic data files do not introduce additional errors of significant amount only the processing codes that passed /16, 37/ the first, second and third rounds of the IAEA nuclear data processing code verification project /16, 37/ were used as shown in Fig.1.

In the comparison of multigroup constants for Th-232 in the unresolved resonance region, we noticed/8/ the following general features: The self shielded cross sections for various energy groups in the unresolved resonance region show a lesser discrepancy than that present in the infinite dilution cross sections. This implies that the discrepancies in basic cross sections have favourably combined with the discrepancies in statistical resonance parameters leading to a lesser discrepancy in self-shielding effects ! This advantage is present only to a lesser extent at the higher temperature 2100 K, where the discrepancy in self shielded cross section is more than the discrepancy at 300 K and approaches that of the infinite dilution cross section.

The magnitude of discrepancy in Doppler changes in self shielded cross sections increases with increasing energy i.e., it is more for higher energy groups. The magnitude of Doppler changes in self shielded cross sections itself decreases with increasing energies for a given data file.

For the multigroup in the resolved resonance region covering the energy region 2040.0 - 3360.0 eV, as shown in Table 1, for Th-232, the infinite dilution capture cross section derived from ENDF/B-V (Revision 2) is found to be larger than JENDL-2 by 39% and the self-shielded cross section(SSCSs) obtained from ENDF/B-V (Revision 2) are larger than those derived from JENDL-2 by a much larger amount i.e. 66.8% at zero dilution going to 39% at very large dilutions. This indicates that the discrepancies in resolved resonance parameters are such as to give lesser discrepancy in infinite dilution cross section but larger discrepancy in self shielded cross section. Further the discrepancy in self shielded cross section approaches the discrepancy in infinite dilution cross section as the dilution approaches a large value. The discrepancy at a dilution of 100 barns in Doppler changes in SSCS for the two data files is about 18% and is much less than the discrepancy in the infinite dilution cross sections.

We have extracted the values of various discrepancies for a dilution of 100 barns that corresponds to a practical reactor composition and assembled them as a function of energy in Table 2 to show the general features at one glance. Table 2 gives an idea of how the two files differ in the characterization of the resonance self-shielding in the resonance region. It should be mentioned that JENDL-2 file adapts the resonance parameter data from the measurements of Rahn et al., /38/ and the resonance parameter data for ENDF/B-V (Revision 2) are those evaluated by Olsen/39/ recently. A reading of the excellent documentation by Olsen/39/ gives the impression to the author that resonance data as recommended by Olsen/39/ and adapted in ENDF/B-V (Revision 2) may be selected for evolving the INDIAN file for Th-232. A final decision on this will be taken in the near future after performing some additional critical survey of literature and comparison studies.

The present ENDF/B convention of using mean resonance parameters in unresolved resonance energy region do not /14-15,40/ lead to a satisfactory treatment of the self-shielding effects in unresolved resonance energy region. A comparison of mean resonance parameters between two files JENDL-2 and ENDF/B-V (Revision 2) for example, may thus turn out to be a mere technical exercise without leading to any physical improvement of the treatment of unresolved resonance region for attaining the goal of better prediction of self shielding effects. The resolved resonance region for Th-232 in the two files extends upto 4keV presently. The considerable structure in capture cross section was parametrized in terms of observed peak positions and areas from 4 to 10 keV in the interesting work of Macklin/41/. The author feels that these /41/ data consisting of observed peak positions and areas may be used advantageously for a more meaningful fitting and recommendation of the statistical resonance parameters in the unresolved resonance region. The formulation of such an interesting work may be taken up at Kalpakkam in the future.

IV. Integral Validation of σ_c and σ_f for Thorium in Fission Source Energy Range

We obtained /4-5,7/ interesting results highlighting the extent to which evaluations in JENDL-2,INDIAN ,ENDF/B-V, ENDL-84, FRENCH SET (1969), INDL/A-83, (RUMANIAN), ENDF/B-IV and JENDL-1 files are consistent with the measured value of for Th-232 at the centre of THOR critical assembly which emphasizes transport of neutrons in the fission source energy range. THOR assembly, in equivalent spherical model /31, 42/ has a core of 5.310 cm radius centered in a reflector of 29.88 cm outer radius. Experimental values of σ_f(U-238) / σ_f(U-235) , σ_f(Th-232) / σ_f(U-238) , σ_γ(U-238) / σ_f(U-235) and σ_γ(Th-232) / σ_γ(U-238) have been published /31/ alongwith the associated uncertainties. We deduced /4-5,7/ the value of alpha from these ratios as 1.9645 $\pm$ 0.146 for Th-232 at core center of THOR assembly.

Shown in Figure 2 are our results for 'C/E' (calculated to experimental ratio) of the value of alpha at the center of THOR assembly. The error in 'C' is taken as 4%, as the uncertainties in cross sections of Pu-239 and those of Th-232 influence 'C' by as much as 4%, on the average, through corresponding uncertainity in calculated neutron energy spectrum. It is clearly seen that the evaluations in ENDF/B, INDL/A-83 (RUMANIAN), JENDL-1 and the FRENCH set overpredict alpha for

Th-232 by 25to 46%. The relative error (in C/E) of 8.43% (4% in 'C' and 7.43% in 'E') could be as large as 11.43% if we treat the error in 'C' as systematic. Then INDIAN and JENDL-2 files are consistent and ENDL-84 and ENDF/B-V would appear, within 5%, consistent with integral measurement of alpha at core center of THOR assembly.

The uncertainty in σ_f for Th-232 in recent files introduce an uncertainty of about 5% in the interpretations of 'C/E' for alpha. The use of recent data of Meadows /35/ for σ_f of Th-232 brings the C/E value to 1.08 for INDIAN file. We therefore conclude that the INDIAN evaluation by Mehta and Jain /19/ for σ_c with σ_f from /35/ and the JENDL-2 for σ_c and σ_f are consistent with the integral value of σ_c/σ_f deduced by us from the measured values of spectral indices at the core center of THOR assembly. Since JENDL-2 uses data of Lindner /43/, for σ_c our analysis validates integrally, Lindner's data. New and accurate measurements of σ_c are needed to reduce further the existing discrepancies 15 - 20% in σ_c (E) for Th-232. Further details are given in /4-5,7/.

The present author, disagrees with the conclusion of ref. /44/ that ENDF/B-IV predicts well the measured capture, fission and (n,2n) reaction rates for Th-232 in fast reactor spectra. The author believes that there might be cancellation of errors in their /44/ particular integral experiment and/or analyses. This opinion is based on the analyses of THOR assembly presented just above. This comment is made to stress that although the mean experimental value may agree with a calculated result, the analyses can lead to valid conclusions only when the uncertainties quoted for experiments and the uncertainties in the calculations together are less than the error in the cross sections that we are testing integrally.. Thus it is desirable to identify and analyse integral experiments that can definitely distinguish and help to quantitatively assess the quality of specific cross sections in specific energy regions in various data files. Our analyses of THOR assembly has been satisfactory in this sense.

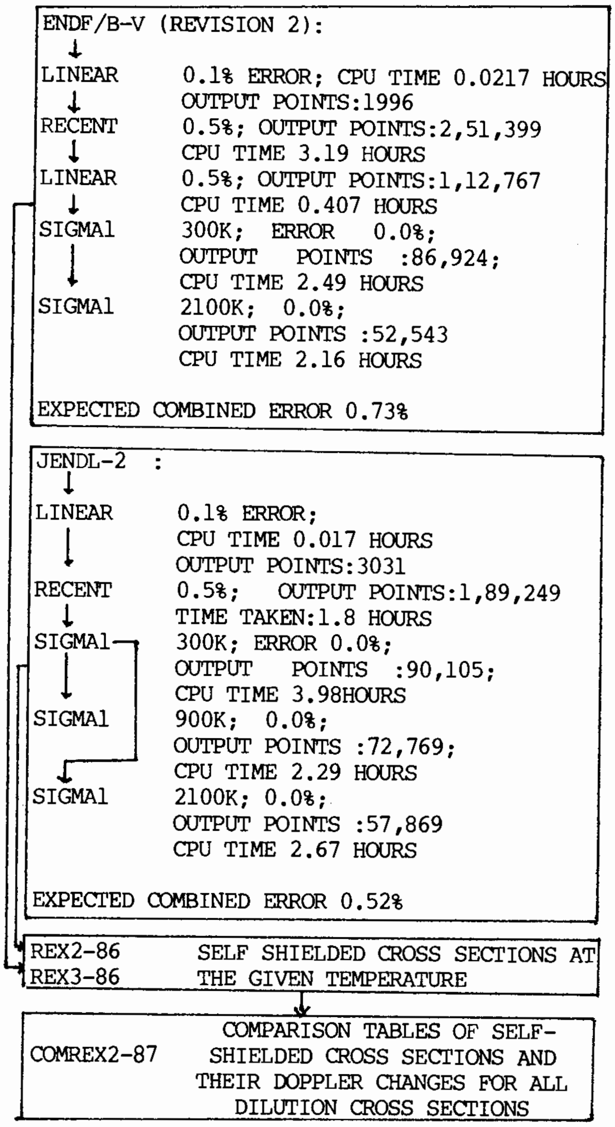

Fig. 1: Calculational flowchart developed at IGCAR, Kalpakkam, for obtaining comparison tables of self-shielded cross sections and their Doppler changes for various dilutions at various temperatures. REX3-86 is for unresolved resonance region.

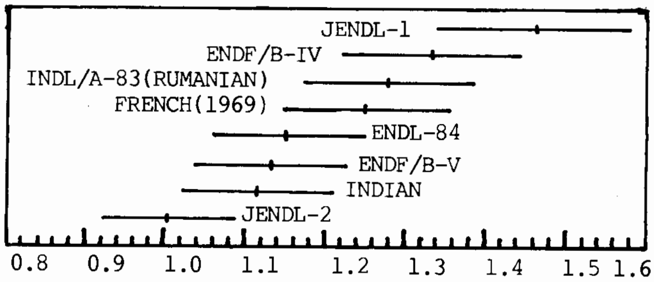

Fig. 2: The comparison of the ratio of calculated to experimental value, "C/E" for various data files for effective "alpha", for Th-232 foil in the centre of THOR assembly. The FRENCH set is described in ref. /61/

V. Integral Validation of (n,2n) Cross Sections for Th-232

The (n,2n) cross sections of Th-232 play an important role in predicting the production of U-232 which leads to hard gamma rays in thorium cycle. We have attempted to intercompare and validate /4, 12/ in an integral sense the (n,2n) cross sections of various available basic data libraries for Th-232.

Experimental values of spectral ratios given at the center of THOR /31,42/ assembly are as follows /31/:

$\sigma_{n,2n}$(U-238) / σ_f(U-238) = 0.053 ± 0.003

σ_f(Th-232) / σ_f (U-238) = 0.26 ± 0.01

$\sigma_{n,2n}$ (Th-232) / $\sigma_{n,2n}$ (U-238) = 1.04 ± 0.03

We cross-multiply and eliminate the cross sections of U-238 and obtain the ratio of experimental value (=E) of effective one group (n,2n) cross section to one group effective fission cross section for Th-232 at the centre of THOR assembly as

$\sigma_{n,2n}$ (Th-232) / σ_f (Th-232) = 0.212±0.0157

This ratio is calculated using various data files and multigroup fluxes at core centre of THOR assembly. The fluxes are calculated using one dimensional transport theory DTF-IV /45/ and the group cross sections $\sigma_{n,2n}$ and σ_f are derived from various basic nuclear data files.

The error in 'C' is taken as 4% in previous section. This coupled with the error in 'E' of 7.4% gives a net error of 8.4% in C/E. The results are given in Table 5.

Except JENDL-2 file all other data files overestimate the $\langle \sigma_{n,2n} \rangle / \langle \sigma_f \rangle$ ratio. The entire (n,2n) contribution comes only from the first group in our present study. From the results presented in the Table 5 we find that JENDL-2 is consistent within the interpretational error bar and the other files show an overprediction of (n,2n) cross section by about 5 to 11% outside the interpretational uncertainty which is assessed to be about 10% (Error of 8.4% plus error in σ_f of JENDL-2) for the last column.

Table 5 Integral Validation of (n,2n) Cross Sections for Th-232

File	Calculated $\langle \sigma_{n,2n} \rangle / \langle \sigma_f \rangle$	C/E	$\langle \sigma_{n,2n} \rangle / \langle \sigma_{f(JENDL-2)} \rangle$ 1 - E Error 10%
ENDF/B-IV	0.283	1.335	1.21
ENDF/B-V	0.255	1.202	1.15
JENDL-2	0.225	1.063	1.06
ENDL-84	0.259	1.221	1.21
INDIAN	0.258	1.22	1.17
INDL/A-83	0.270	1.275	1.18

VI. Analysis of Central Reaction Rates for Th-232 in CFRMF Assembly

In the analysis of CFRMF it is stated /46/ that the integral measurement of Th-232 (n,γ) at CFRMF is inconsistent with ENDF/B-IV data and that the capture cross section for Th-232 should be adjusted upwards by 10% in 0.1 keV - 1 MeV energy region. At 23 keV measurements of Baldwin and Knoll /47/ is consistent with this observation. This is in contradiction in 800 keV to 1 MeV energy region with our results /4,7// based integral validation of $\langle \alpha \rangle$ for THOR assembly that ENDF/B-IV overestimates $\langle \sigma_c \rangle$ in 800 keV - 4 MeV energy region. The discrepancy can be resolved if we note that CFRMF covers /46/such a wide energy region than THOR /31,42/which covers just the fission source energy range.

Results of our calculations of central reaction rates for Th-232 in CFRMF using the BNL/31/ Benchmark specification for 620 group flxes are presented in Table 6.

Table 6 Integral cross section (mb) at core of CFRMF assembly

REACTION	MEASURED/31,46/	CALCULATED AT IGCAR ENDF/B-V(Rev.2)	JENDL-2
Fission	19.6 $\pm$5.2%	19.15	20.10
Capture	290.0 $\pm$3.8%	257.98	239.42

The inference is that the $\langle \sigma_c \rangle$ values in ENDF/B-IV are underpredicted by not just about 10% as indicated /46/ by CFMRF analysis in 100 ev to 800 keV energy region but some percent more than 10% as we have to provide for cancellation of higher $\langle \sigma_c \rangle$ values in ENDF/B-IV in 800 keV to 1 MeV energy region.

VII. System criticality considerations for U-233 metal assembly

The critical assembly JEZEBEL-23 as a bare sphere of U(98.13 at/w% U-233) metal, is especially suited /31/ for testing U-233 cross sections in the fission source energy range. The reactor region cross sections were prepared using EFFCROSS code /48/ and the one dimensional transport calculations in spherical geometry were performed using DTF-IV code /45/. The results are presented in Table 7. Very interestingly both the recent files ENDL-84 and JENDL-2 libraries predict K-eff within 1%. Note that the French set (1969) over-predicts K-eff by 3.76% whereas ENDF/B-IV based multigroup set underpredicts K-eff by as much as 3.2%. Thus a spread of nearly 6.94% exists in the calculated values of K-eff for the U-233 system calculated from these two older files.

In the present analysis of JEZEBEL-23 critical assembly the most important groups contributing to capture and fission reaction rates are in 500 keV - 3 MeV energy region. From all the results of intercomparison /9/ we conclude that the higher calculated value of K-eff obtained by the use of the French set is mainly explained by the fact that the French set has higher σ_f values. The lower value of K-eff calculated by ENDF/B-IV is explained to be mainly due to the lower value of σ_f in ENDF/B-IV. Complete details of this study have been documented /9/ and a comparison of σ_c and σ_f for U-233 is presented in Table 3 and Table 4.

Table 7 System criticality considerations for U-233 metal assembly

Measured Eigen Value : 1.000 $\pm$ 0.001 /31/

Case	File Used For U-233	K-eff, Calculated
1	French (1969)	1.0374
3	ENDF/B-IV	0.9682
4	ENDL-84	1.0072
5	JENDL-2	1.0008

VIII. Analyses of U-233 irradiation experiment in the experimental fast reactorRAPSODIE

This section summarises results of calculations performed for analysis of U-233 irradiation experiment conducted in RAPSODIE reactor/32/. In Table 8, we present the effective fission and capture cross sections calculated using the four different multigroup sets and also the data of Meadows/36/ for fission cross section. There is relative consistency in the "C/E" value of effective fission cross sections of the French "TACO" experiment presented in Table 8 and of K-eff of JEZEBEL-23 assembly. The reported /32/ experimental value of fission cross section in Table 8 has an error of + 6%. Thus a "C/E" of 0.95 is well within this error of 6%, thus making the analysis less effective. Unfortunately, therefore, this integral validation study cannot strictly claim to lead to any definite recommendation on U-233 fission or capture cross sections. We are inclined to suggest that probably due to poor characterisation of neutron spectra the calculated effective cross sections may have a systematic error. The experiments proposed by Demeester et al., /49/ are expected to avoid the weaknesses of the "TACO" experiment by characterizing the neutron spectrum accurately at the irradiation position.

Table 8 Integral cross sections (in barns) for U-233 in RAPSODIE reactor

	FISSION	CAPTURE
Experimental values (E) /32/		
(RAPSODIE)	2.31 ± 6%	0.155± 0.2%
Calculated values (C)		
KEDAK /32/	2.12	0.155
C/E	0.92	1.0
CADARACHE (IGCAR)	2.28	0.182
C/E	0.99	1.17
ENDF/B-IV /32/	2.11	0.156
C/E	0.91	1.01
ENDL-84 (IGCAR)	2.195	0.164
C/E	0.95	1.06
JENDL-2 (IGCAR)	2.141	0.165
C/E	0.93	1.065
MEADOWS (IGCAR)	2.196	-----
C/E	0.95	-----

IX. Scope for further work in the development of INDIAN cross section data file

A possible improvement for Th-232 under active consideration is the following at present.

The reports in the literature have not yet converged to unique recommendations for the data of inelastic scattering cross sections for discrete levels and their angular distributions for Th-232. For example, the measured Time-Of-Flight spectrum from the one mean free path Th-232 sphere pulsed with 14 MeV neutrons was predicted /50-51/ better with ENDF/B-V data as compared to ENDF/B-IV data. The K-eff analysis presented /4/ for THOR assembly indicated that the INDL/A-83 /34/ file for Th-232 predicted K-eff better when its inelastic cross section data was substituted with inelastic cross section data taken from JENDL-1 file. However the inelastic cross section data of Th-232 in JENDL-1 file has been considerably changed in JENDL-2 /28-29/ version. The recent work of Chawla et al., /52/ shows that the measured flux spectra in thorium blanket of PROTEUS assembly was predicted with ENDF/B-IV data well between 30 and 500 keV but overpredicted at higher energies. The spectra in spherical thoria pile measured by Block et al., /53/ and Feigenbaum et al.,/54/ was predicted better with ENDF/B-V data. Except below 4 MeV, the ENDF/B-IV file could predict the neutron spectrum measurement with a thoria blanket mockup at the ORNL tower shielding facility according to Ingersoll et al., /55/. The recent reports from Kyoto team /56/ indicate that the transmitted spectra both from spherical thoria pile and metallic thorium slab are predicted better with ENDF/B-V and JENDL-2 only when the inelastic data from ENDF/B-IV are substituted in these files. The work of Smith and Guenther /62/ on differential measurements suggests that Th-232 total-inelastic-scattering cross sections over the incident energy range 1.0-3.5 MeV involving energy transfers of more than several hundred keV as given in ENDF/B-V data /57/ are correct to within the respective uncertainties. According to Smith and Guenther /62/ the improvements in the understanding of inelastic scattering from Th-232 should probably focus upon a better determination of energy transfer within an essentially fixed total-inelastic-scattering cross section. The recently measured /58/ value of inelastic scattering cross section at 144 keV using Si-filtered neutrons at the University of Missouri Reasearch Reactor was higher than the value in INDL/A-83 and ENDF/B-V files and is in agreement with JENDL-2 file. In summary, there is considerable confusion in the results of integral validation of inelastic cross sections for Th-232 in the literature. We believe that there is a need to re-perform some of the integral tests for validation of inelstic cross sections. We clearly recognize that the inelastic cross sections for discrete levels and their angular distributions need to be critically intercompared, examined and validated. The recent data provided by the Lowell group's theoretical and experimental evaluations /59/ and those of Oxford team /60/ do not favour ENDF/B-V data especially in the case of more highly excited levels.

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