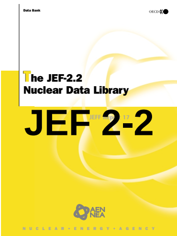

BENCHMARK CALCULATIONS FOR URANIUM 235

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ABSTRACT

The neutron capture to fission ratio (α) in the resonance range for ^{235}U is currently believed to be about 0.5. Small variations have significant effects on the predicted criticality of thermal reactors and fuel storage/transport configurations. Unfortunately α is highly dependent on incident neutron energy and it is necessary to assess evaluations by comparing calculated predictions of criticality with experimental measurement over a wide range of neutron spectra. This paper is an assessment of the latest evaluations produced in an international programme initiated after noting that the resonance capture in ENDF/B-VI and JEF2.2 seemed too small.

I. INTRODUCTION

The JEF2.2 and ENDF/B-VI Benchmark Programmes have suggested that the JEF2.2 and ENDF/B-VI revision 2 nuclear data evaluations contain too little resonance capture for ^{235}U[1,2]. As a result, new evaluation work has produced a file adopted for the Joint Evaluated Fission and Fusion library version 3 (in its Test status) JEFF-3.T. The evaluation work is organised by Sub-Group 18 of the OECD NEA Working Party on Evaluation Co-operation. Various ^{235}U evaluations have been released in revisions of ENDF/B-VI and the file proposed for ENDF/B-VI revision 4 was initially suggested for inclusion in JEFF-3.T. The file is described in JEF/DOC 552[3] and was issued, in January 1996, to international evaluators for comment.

Moxon examined the January 1996 Leal, Derrien et al evaluation using his REFIT[4] code and issued a paper proposing improvements[5]. These were discussed at the July 1996 JEF meeting. As a result, a collaborative evaluation exercise took place at Oak Ridge National Laboratory, USA (ORNL). An evaluation was produced in December 1996 but was not made available in Europe until March 1997[6].

Further study by sub-group 18 and benchmark testing in the USA resulted in the issue of a further evaluation in October 1997[7]

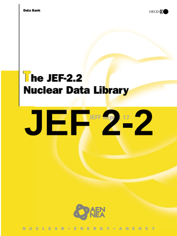
This paper describes the use of these ^{235}U evaluations in suitable benchmark studies.

II. COMPUTER CODES AND METHODS

All benchmark calculations used the Monte Carlo code MONK8[8]. For each assembly, three calculations were run. Each used different initial random numbers. Convergence criteria were adjusted to fit each case and to predict k_{eff} to within a standard deviation (σ) of 80pcm ($\Delta_k \times 10^5$). No other physics parameters were considered in this study. Calculations were performed using both point and broad grouping of incident neutron energy dependence as noted below.

III. APPLICATIONS LIBRARIES

Standard nuclear data libraries for MONK8 are produced from JEF2.2 evaluated nuclear data[9]. All nuclide data on the 1996 DICE library[10] for MONK8 are modelled in 13,193 hyper-fine energy groups. A pre-shielding treatment is also applied for major fuel isotopes and structural materials. This treatment includes fitting shielded data averaged over 4 (Δu=1/960) groups for U238 and 2 groups for ^{235}U. The 172 group 1996 WIMS nuclear data library[11] was used within MONK8 throughout the broad group work. Resonance shielding is



...uded for major fuel isotopes and absorbers in the form ...abulated resonance integrals in the energy range 4eV ... KeV. It is applied using a sub-group treatment[8].

The JEF2.2 ^{235}U data were already present on the libraries. The NJOY Code[12] had been used to generate these data and has also been used to process all other ^{235}U evaluations. All processed data were added to the libraries as extra nuclides.

IV. ^{235}U EVALUATIONS

This benchmark testing uses six versions of ^{235}U evaluated nuclear data. JEF2.2 and ENDF/B6 revision 2[13] were the starting points for the benchmarking programmes in Europe and the USA respectively. Studies using these evaluations indicated problems attributed to too little resonance capture in ^{235}U[1,2]. Attention has been concentrated on the resolved resonance and thermal ranges.

ENDF/B-VI revision 3[14] was the first attempt to rectify the situation. In this revision the mean capture width below 100eV was increased from ~33meV to ~37meV. The resolved resonance range remained sub-divided into 11 bands with extra unphysical resonances inserted, allowing a continuous cross section to be generated from reasonably quick NJOY processing.

The next proposed evaluation was issued in January 1996[3]. The mean capture width below 100eV was ~45meV but there was considerable variation in individual resonances. A single energy band was used in the resolved range. This removes the unphysical resonances but significantly increases the NJOY processing time. This is the file assessed by Moxon. The assessment resulted in a collaborative study at ORNL.

A preliminary evaluation[6] resulted from the ORNL study completed in December 1996. Limitations have been placed on the variation of the capture width in the range 4 to 100eV by setting widths smaller than 30meV and larger than 60meV, to 40meV. However several resonance widths had to be reset in order to obtain suitable fits to experiment when the SAMMY[15] code was used. At higher energies a mean width of 40meV was used with a 2% constraint.

Further evaluation work took place in the US using SAMMY and resulted in a file suggested for inclusion in ENDF/B-VI revision 5 and adopted for JEFF3.T[7]. It included fitting of more experiments, introduction of some integral parameters and changes to number of neutrons per fission in the thermal range. The mean capture width is 38.03±1.70 below 50eV. There remain divergent values but these can be traced to large fission resonances and the capture discrepancy tends to be within the overall error. Moxon has confirmed the width by using REFIT to attain a consistent capture width of 38.13meV which he applied up to 130eV[16].

V. ^{235}U BENCHMARKS

The effect of using the January 1996 ^{235}U evaluation[6] instead of JEF2.2 for more than 60 experiments was studied by S. Cathalau, P. Blaise[17]. Surprisingly they found JEF2.2 gave better agreement with experiment. However, when the same experiments used in Cathalau's initial study[1] were considered, the January 1996 evaluation gave improved results! The JEF meeting concluded that it was important to carefully select experiments and always to use reference codes (Monte Carlo if possible).

Rowlands considered the problem of benchmark selection[18]. Based on his selection ideas and taking account of cases considered in the USA, ten benchmarks have been selected in an attempt to cover a full range of intermediate and thermal neutron spectrum systems. Benchmarking in the USA had used the HISS Uranium assembly from the Hector reactor at Winfrith[19] together with the two TOPSY reflected Uranium hydride assemblies UH3Ni and UH3UR[20]. All three have hard spectra. The hardest and softest ORNL spheres[21] are included together with the hardest and softest Uranium fluoride critical experiments: UF1 and UF6[22]. DIMPLES01[23] and TRX[21] are both Uranium fuelled lattice benchmarks with good specification data in the public domain. A single VALDUC UO_2 lattice[24] criticality case is also considered.

VI. RESULTS

Results consist entirely of k_{eff} predictions from the Monte Carlo code MONK8. At this stage we have not performed analysis of experimental and modelling errors since we are viewing trends with respect to the changing ^{235}U evaluations. Only ^{235}U data were changed between runs; all other nuclear data are taken from JEF2.2 without adjustment.

Results were obtained by tracking in continuous energy taking data from the 13,193 hyper-fine energy group library. k_{eff} predictions from each of the three runs are averaged together with their "1 σ " standard deviations. These are obtained from:-

$$\overline{\sigma} = \frac{1}{\sqrt{\sum_{j=1}^{3} 1/\sigma_j^2}} \ .$$

The experimental result is then compared and values of Calculation minus Experiment relative to Experiment ((C-E)/E) produced in terms of pcm (relative $k_{effective}$ difference$\times 10^5$). Results are given for the six evaluations: J2U235 indicates JEF2.2; E6R2U235 refers to revision 2 of ENDF/B-VI, E6R3U235 specifies ENDF/B-VI revision 3, E6DU235 indicates the January 1996 evaluation of Derrien et Al, E6ORU235 indicates the December 1996 preliminary evaluation from the ORNL study and finally E6R5U235 indicates the latest evaluation issued in October 1997 and adopted for JEFF3.0.

Results were also obtained using the 172 group 1996 WIMS nuclear data library. These are performed using the same structure.

In order to compare (C-E)/E values from various countries, the JEF project suggests results be tabulated against “q”:- the number of fission neutrons reaching 2.6eV. (Sometimes 4eV is used but it makes little difference.) A low value of “q” represents a hard spectrum; the softest system, with no resonance absorption, has a “q” of 1. The values of “q” used in the rest of the report were calculated from the J2U235 MONK8 results. We tabulate all further results accordingly.

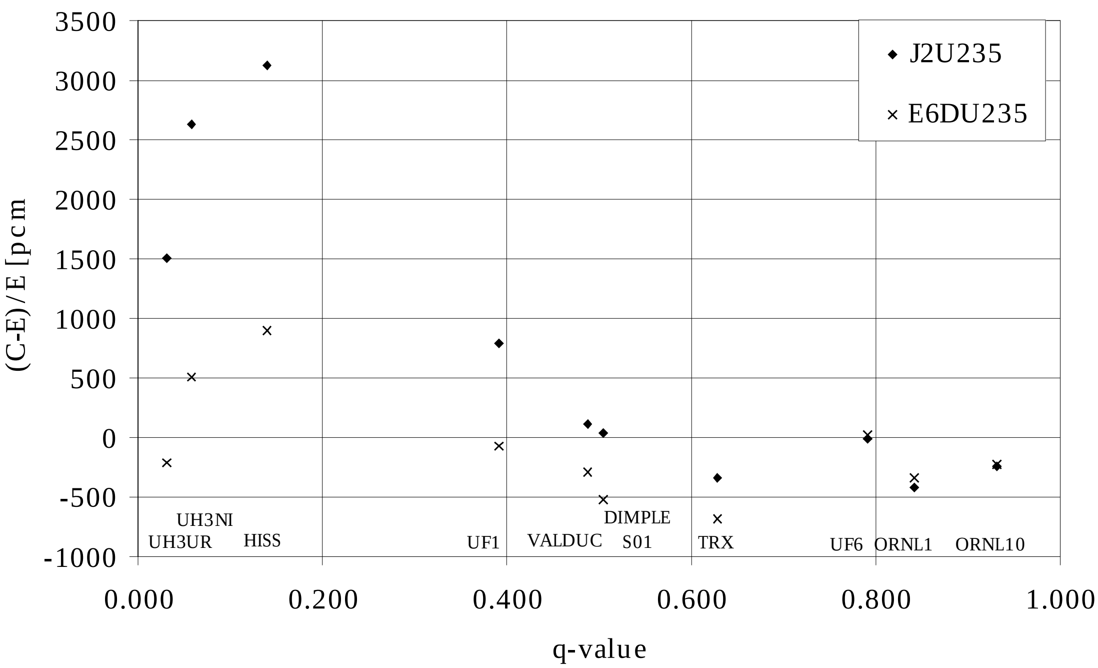
The first table, below, compares broad and hyper-fine group results as predicted using JEF2.2.

Benchmark	q-value	Hyper-Fine (C-E)/E	Broad (C-E)/E	Δ
UH3-UR	0.031	1643	1637	7
UH3-NI	0.058	2577	6057	-3480
HISS (HUG)	0.141	3103	2837	267
U fluoride 1	0.391	700	593	107
Valduc - MONK2.01	0.488	27	-247	273
DIMPLE Assembly S01	0.503	-93	-73	-20
TRX1	0.628	-580	-777	197
U fluoride 6	0.792	20	-150	170
ORNL1	0.843	-370	-583	213
ORNL10	0.932	-217	-493	277

The first two columns describe the case and spectrum softness. Hyper-fine group relative predictions of k_{eff} are followed by broad group results. Both are given in terms of pcm. Differences (Δ) are then listed. If we consider an overall convergence for two samples with standard deviations $\sigma \approx 80$pcm, we get $\sqrt{2}\sigma$ to be ~110pcm between the hyper-fine and broad results. All but one case compare with experiment within $3(\sqrt{2}\sigma)$. The Ni reflected TOPSY result indicates that broad group methods cannot be applied due to the high energy resonance structure. Even if resonance shielding was applied, it would be very difficult to model, due to large variation over short distances at the inside edge of the reflector. Our conclusion is that fine group data are needed. Since this assembly is used in the American ^{235}U benchmark studies, we did not wish to find a substitute due to a method restriction.

All further analysis in this report will use the hyper-fine group results listed in the next table.

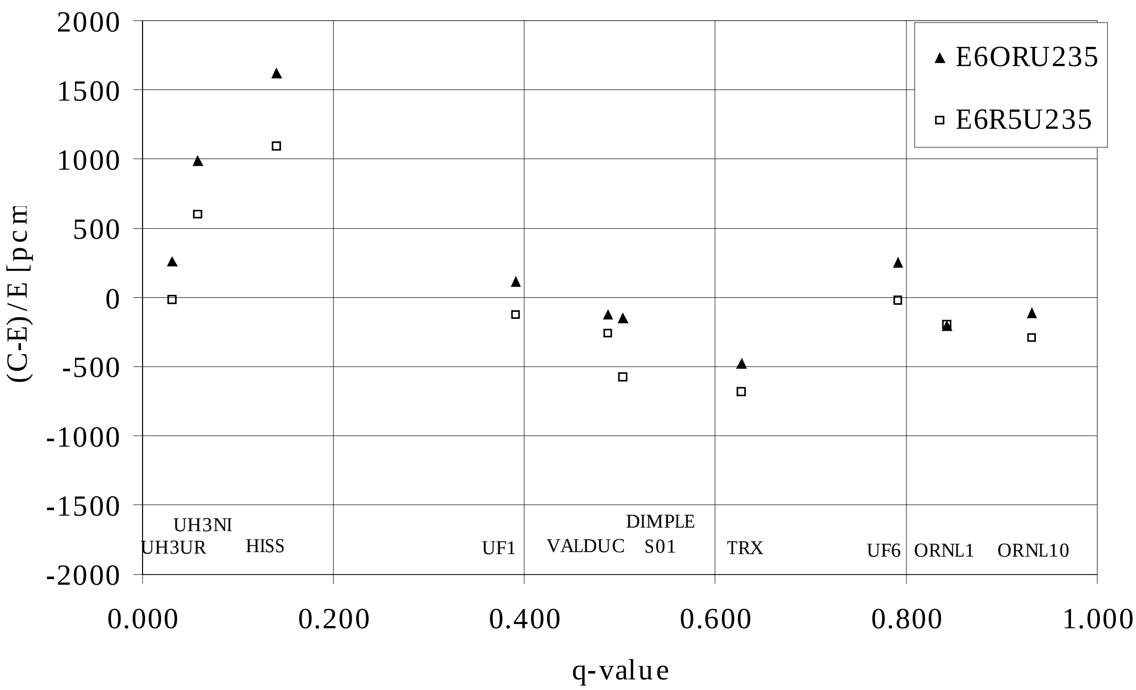
Benchmark	q-value	MONK8 - Hyper fine -K_{eff} (C-E)/E					
		J2	E6R2	E6R3	E6D	E6OR	E6R5
UH3-UR	0.031	1643	1637	327	-180	257	-17
UH3-NI	0.058	2577	2747	1093	563	987	600
HISS (HUG)	0.141	3103	2980	1360	867	1620	1090
U fluoride 1	0.391	700	573	-37	-247	110	-127
Valduc - MONK2.01	0.488	27	-3	-250	-300	-127	-260
DIMPLE Assembly S01	0.503	-93	-213	-327	-473	-150	-577
TRX1	0.628	-580	-613	-637	-777	-480	-683
U fluoride 6	0.792	20	90	150	-47	250	-23
ORNL1	0.843	-370	-177	-143	-240	-207	-200
ORNL10	0.932	-217	-247	-93	-153	-114	-292



This first figure compares JEF2.2 (J2U235) results with those from the January 1996 evaluation(E6DU235).

This comparison shows the most radical change in the prediction of k_{eff}. It is worth noting that two gaps can be in the range of experiments studied as well as some lap between DIMPLES01 and VALDUC. We could rove the analysis by finding systems with a "q" between 0.2 and 0.4. However, the main trend is that the increased capture in the January 1996 evaluation has significantly improved the three hard spectrum assemblies. It is important to question whether the initial rise in $k_{effective}$, seen with the January 1996 evaluation, with increasing q is random or indicative that systems similar to HISS are still predicted at about the 1% super-critical level. Throughout the ^{235}U evaluation work, the unresolved data have not been changed. Average resonance parameters in the unresolved range are normally developed by studying the behaviour of resolved parameters with increased incident neutron energy. This has not been done yet. It may be worth optimising an evaluation in the unresolved resonance range and investigating the impact on the hard assemblies before continuing with more in-depth analysis at lower energies.

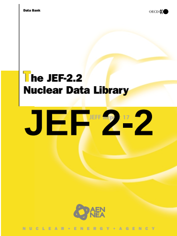
With the three hard systems removed, all calculations except UF1 predict k_{eff} within ~0.5% (500pcm) using JEF2.2. DIMPLES01 and TRX are outside 0.5% with the January 1996 evaluation. There is little difference between evaluations for the soft assemblies (q above 0.8). Unfortunately DIMPLES01 is very important being similar to a PWR in terms of neutron spectrum.



This second figure above compares results for the two latest evaluations which have been developed since the benchmarking of JEF2.2 and ENDF/B-VI revision 2 indicated the need to increase ^{235}U resonance capture. The overall improvement from JEF2.2 can be seen by the lack of points above 1620pcm. The trend observed with the December 1996 ORNL evaluation is back towards ENDF/B-VI revision 3 results (see table). Although it has been said that the hard spectrum assemblies are still over-predicted, this is indicated by only two out of the three assemblies. The results for UH3UR are now VERY good! The question raised earlier regarding the hard spectra is even more valid now that HISS results are ~1600 pcm high.

The ENDF/B-VI revision 5 ^{235}U evaluation has improved the results for the three hard spectrum systems. Results are almost within ~1% and the most improvement is seen for the most discrepant system (HISS).

Unfortunately, if one excludes the three hard systems, the latest evaluation reduces all results which already seemed underpredicted. In this range the December ORNL evaluation seems the best! One could conclude that all results except TRX were within ~250pcm of unity



n these data are applied. This is no longer true with ENDF/B-VI revision 5 ^{235}U evaluation where results oth TRX and Dimple are unacceptably low.

VII. CONCLUSIONS

1. A study of the impact of new ^{235}U evaluations has been completed.
2. The use of selected high-quality benchmarks is required.
3. The use of MONK8 with hyper-fine group data predicts trends effectively.
4. Broad group analysis is not suitable for Ni reflected assemblies.
5. Broad group trends are similar to fine group trends for other systems.
6. The impact of changes to data in the unresolved ranges should be considered.
7. Very good results are now obtained for one hard system - UH3-UR.
8. Results with the 1996 ORNL evaluation are within 250 pcm for seven of the ten assemblies.
9. The latest ENDF/B-VI revision 5 (=JEFF3.T) gives the best results for the three hard systems but at the expense of important thermal systems.
10. Improvements are still needed to the ^{235}U evaluations.

ACKNOWLEDGEMENTS

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REFERENCES

1 S Cathalau, A Benslimane, A Maghnouj, P. Fougeras, and V. Ukraintsev
"Qualification of the JEF2.2 Cross-Sections in the Epithermal and Thermal Energy Ranges Using a Statistical Approach"
P101, Vol. II 1994 Topical Meeting on Advances in Reactor Physics, Knoxville, TN April 11 - 15 1994.

2 A. C. Kahler
"Homogeneous Critical Monte Carlo Eigen-value Calculations with Revised ENDF/B-VI Data Sets"
P 384 1995 Annual Meeting Philadelphia, Pennsylvania June 25 - 29, 1995
Transactions of the American Nuclear Society Volume 72 TANSAO 72 1-408 (1995) ISSN:0003-018X

3 L. C Leal, H. Derrien, R. Q. Wright and N. M. Larson
"Final Report on Evaluation of the ^{235}U Cross Section"
JEF/DOC -552
January 10 1996

4 M C Moxon
"REFIT A Least Square Fitting Program for Resonance Analysis of Neutron Transmission and Capture Data"
AEA-InTEC-0470
1986

5 M C Moxon
"REFIT Calculation of the Latest ENDF/B-VI ^{235}U Resonance Parameters"
JEF/DOC-617
1 July 1996

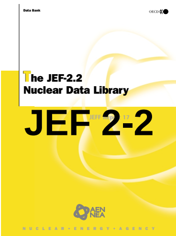
6 H.Derrien, L.Leal, N.M.Larson, M.C. Moxon
"Problems Related to the Resonance Analysis of ^{235}U"
JEF/DOC-627

7 L.C. Leal, H. Derrien, N.M. Larson, R.Q. Wright
"R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 eV to 2.25 keV"
ORNL/TM-13516 (1997)

8 M J Armishaw, J L Hutton, N R Smith and J Sidell
"Features of the Monte Carlo Code MONK8"
This Conference

9 C Nordborg, H Gruppelaar and M Salvatores
"Status of the JEF and EFF Projects"
Page 782 of Proceedings of an International Conference on Nuclear Data for Science and Technology held at the Forschungszentrum Juelich Fed. Rep. of Germany
13-17 May 1991

10 C R Eaton, M J Grimstone



"The 1996 DICE Nuclear Data Library"
AEAT-0269
March 1996

11 C J Dean, R J Perry
"The 1996 WIMS Nuclear Data Library"
AEAT-0293
March 1996

12 R E MacFarlane, D W Muir
"The NJOY Nuclear Data Processing System Version 91"
LA-12740-M
October 1994

13 P F Rose (editor)
"ENDF-201 ENDF/B-VI, Summary Documentation"
BNL-NCS-17541
4th Edition
October 1991

14 C R Lubitz
"A Modification to ENDF/B-VI U-235 to Increase Epithermal ALPHA and K1"
Proceedings of the International Conference on Nuclear Data for Science and Technology, Gatlinburg, Tennessee
May 9-13, 1994

15 N.M.Larson
ORNL-TM-9179/R1(1985),/R2(1989),/R3(1996).

16 M.C.Moxon
"An Evaluation of the ^{235}U Resonance Parameters using the Program REFIT".
JEF/DOC-708

17 S. Cathalau, P. Blaise
"Synthesis of the Comparison of JEF-2.2 (ENDF/B-VI) and LEAL-DERRIEN/95 Evaluations for ^{235}U"
JEF/DOC-589

18 J.L. Rowlands
"Benchmarks for Validating U-235 Resonance and Thermal Region Evaluations. Some Initial Proposals"
JEF/DOC-624
16 September 1996

19 H H W Pitcher, J E Sanders, V G Small
"An Experimental Study of the Integral Properties of U235 and Pu239 in an Intermediate Energy Spectrum, and Comparison with Theoretical Prediction"
AEEW - R 566
March 1968

20 G A Linenberger, J D Orndoff, and H C Paxton
"Enriched-Uranium Hydride Critical Assemblies"
Nuclear Science and Engineering: 7, 44-57 (1960)
September 25 1959

21 "ENDF-202 Cross Section Evaluation Working Group Benchmark Specifications"
BNL 19302
November 1974 updated to September 1991

22 N.Smith, A. Nouri
"Inter-code Comparisons for Highly Enriched Uranium Fluorine Benchmarks"
JEF/DOC-596
July 1996

23 R.J. Perry, C.J. Dean
"DIMPLE S01A Models"
JEF/DOC-518
March 1995

24 D Hanlon
LEU-COMP-THERM007
"International Handbook of Evaluated Criticality Safety Benchmark Experiments"
NEA/NSC/DOC(95)03
1996