IEC-143

SYNTHESIS OF THE COMPARISON OF JEF2.2 (ENDF/B-VI) and LEAL-DERRIEN/95 EVALUATIONS FOR ^{235}U.

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1. Introduction.

In several recent studies, it has been demonstrated that the resonance region evaluation of ^{235}U (of Leal and de Saussure) adopted in both the US (ENDF/B-VI) and Western European (JEF2.2) nuclear data files, is unsatisfactory wrong especially for the capture cross-section in the resolved resonance energy range. These studies have shown that, while the fission cross-section seemed to be correct over the whole energy range, an underestimation of about 10 % to 13 % has been found for the capture cross-section in the resonance energy range.

An investigation of the evaluated data file concluded that the probable explanation was an underestimation of the mean capture width (by about 10 %).

This is a reason why several studies have been undertaken in the US in order to produce a new resonance region evaluation for the ^{235}U isotope : a recent evaluation by LEAL and DERRIEN (1995) is now available : several studies are now in progress in Europe and the USA to quantify the benefits of this new evaluation.

This paper summarizes the studies performed at CEA Cadarache (France) devoted to the LEAL-DERRIEN tests in LWRs lattices. The first section compares the multigroup cross-sections for an infinite dilution in the JEF2.2 and the LEAL-DERRIEN evaluations. The second section describes the code and the experimental benchmarks which have been used for benchmarking the new evaluation. The third section is devoted to the results of this benchmarking.

2. Comparison of the JEF2.2 and LEAL-DERRIEN evaluations.

In the LEAL-DERRIEN evaluation, cross-sections between 0 eV and 2250 eV are represented by about 3170 resonances. Fourteen bound states have been added in order to determine the shape of the cross-section in the thermal energy. Above 2250 eV, fourteen levels have been added in order to simulate the contribution of all the resonances which are located at higher energies. These 28 fictitious levels give a very good representation of the potential cross-section in each considered energy range.

In this evaluation, a unique scattering radius has been used over the whole energy range. This radius was deduced from the analysis performed by SAMMY of the experimental data related to the transmission measurements of Harvey.

Figures 1 to 4 give the differences between JEF2.2 (and ENDF/B-VI) and the LEAL-DERRIEN new evaluation. The infinite dilution cross-sections have been reconstructed using the NJOY code with a flat weighting spectrum. We can note that in the low thermal energy range (0 eV - 0.1 eV), the evaluations are very similar (differences about or lower than 3 %, except for the scattering cross-section). For the fission or the capture cross-section. very large differences can be noted for each resolved resonance (from 0.3 eV until 2250 eV) : for example, the fission cross-section is decreased by about 5 % and the capture by about 10 % in the first resonance at 0.32 eV in the LEAL-DERRIEN evaluation. We can also note differences up to about + 18 % for the fission cross-section (4 eV) and by about 37 % for the capture (700 eV).

Figure 5 presents the discrepancy for the ratio « fission/capture » between the two evaluations : it is shown that the LEAL/DERRIEN-95 evaluation is very much lower than the JEF2.2 evaluation and consequently, the multiplication factors calculated with the new evaluation will be smaller than those obtained with JEF2.2 : the effect due to the decrease of the fission cross-section is added to the effect due to the increase of the capture cross-section.

This first analysis indicates that, while the modification of the capture cross-section seems to go in right direction, the strong modification of the fission cross-section could induce unexpected effects on the multiplication factor of thermal lattices.

These tests are presented in the following section.

3. Benchmarking calculations.

3.1 Description of the code and library.

For this study, we have used the APOLLO-2 code which is the latest version of the lattice code for thermal reactors. It has been developed over the past ten years : it is completely modular and a specific user friendly language is used. It solves the Boltzmann equation with the multigroup approximation using collision probability methods.

Specific self-shielding methods have been developed which calculate the effective reaction rates (and self-shielded cross-sections) with very low discrepancies compared to results obtained using MONTE-CARLO reference methods.

We have used APOLLO-2 as a reference code for the comparison of calculated neutronic parameters obtained with both JEF2.2-^{235}U (or ENDFB-VI) and LEAL/DERRIEN-^{235}U evaluations (the data for the other nuclides remained the same).

We used the CEA93 library in 172 groups this being completly based on JEF2.2 evaluations. The multigroup cross-sections were obtained using the NJOY code using appropriate weighting spectra.

3.2 Brief description of the investigated experiments.

The studies performed at CEA in 1993, which showed the error in the epithermal range for the ^{235}U capture cross-section (JEF2.2), were realized using few (about 10) experiments involving ^{235}U : however, it was concluded at the time that more experiments should be analysed.

Consequently, during the present study, we have investigated a wider range of available experimental results involving ^{235}U. Thus, several experimental programs have been calculated. Table I gives an overview of the experiments, which involve metallic uranium fuel and UO_2 fuel, both H_2O and D_2O moderators, stainless steel, aluminium or

Zircalloy cladding materials, hexagonal and square pitches. Spherical uranium nitrate experiments have also be calculated. These experiments were performed in several countries.

4. Results of the calculations.

TABLE II summarizes the k_{eff} values obtained using the APOLLO-2 code for the chosen experiments with both JEF2.2 and the LEAL/DERRIEN evaluation. A slight underestimation of the calculated K_{eff} is indicated for the calculations using ^{235}U from JEF2.2 (Averaged E-C = + 105 ± 625 pcm), and this underestimation is greater when the LEAL/DERRIEN evaluation is used (Averaged E-C = + 411 ± 680 pcm). The differences between calculated K_{eff} values obtained using JEF2.2 and the LEAL/DERRIEN evaluations are plotted in fig. 6. It can be seen that the difference decreases with the slowing-down density (number of neutrons which are absorbed below 4 eV) : the ^{235}U resonance region capture rate is more sensitive for « under-moderated » experiments in which the epithermal spectrum is higher than in standard PWR lattices : for example we can observe a difference of about 730 pcm for the CRISTO experiment (q = 0.36) and differences between 0 pcm and -34 pcm for the D_2O experiments (q ~ 0.7 to 0.9). This trend is completly consistent with the modification of cross-sections between JEF2.2 and the LEAL/DERRIEN evaluations which have been discussed in the previous section.

However, if we refer to the experiments which were investigated in 1993 (TABLE III), we can conclude that the new evaluation gives better results than the previous one.

Another test which has been made is of the ^{235}U capture rate relative to ^{235}U fission rate, which has been measured during the SHERWOOD programme. The results are as follow:

^{235}U JEF2.2 calculation : (E-C)/ C = + 5.4 ± 3.0 % (2σ).
^{235}U LEAL/DERRIEN calculation : (E-C)/ C = + 4.4 ± 3.0 % (2σ).

This result shows that the new evaluation gives a better prediction than the older (JEF2.2) one, but the experiment/calculation discrepancy remains.

In addition to this work, a specific study has been performed comparing the sensitivity coefficients of K_{eff} to ^{235}U cross-sections obtained for both evaluations. The differences between the sensitivity coefficients calculated in 15 macrogroups (TRX2 experiment) are shown in figure 7. It is indicated that the sensitivity coefficients are drastically modified (between + 4 % and + 16 %) in the energy range of interest (0.1 - 1 keV) : a specific investigation of these effects must be performed in order to understand what happens in these calculations (it is usually assumed that the sensitivity coefficient does not change significantly with the cross-section data set).

5. Conclusions.

This work is devoted to the benchmarking of the new evaluation « LEAL/DERRIEN-95 » for ^{235}U which has been completed recently because some studies have demonstrated that the previous evaluation gave poor results for Uranium fuel in thermal reactors : the capture cross-sections seemed to be underestimated by about 10 % to 13 % in the epithermal energy range but the fission cross-section in the JEF2.2 evaluation appeared to be good.

This study began by a comparison of the multigroup (172 groups) cross-sections obtained using NJOY : the observed differences for the capture cross-section were consistent with the changes found to be required during the benchmarking of JEF2.2 but the differences for the fission cross-sections seem to be to high : consequently it could be concluded that the multiplication factors obtained using the new LEAL/DERRIEN evaluation would be smaller than those obtained using JEF2.2.

This has been demonstrated during the benchmarking which has used more critical experimental results than previously studied. The observed effects on k_{eff} are consistent with the modifications of the evaluated cross-sections (increase of the capture cross-section and decrease of fission cross-section). However, it is very difficult to conclude at this stage of the study which evaluation is better.

In particular, the averaged E-C using our calculational scheme with the LEAL/DERRIEN evaluation goes in the wrong direction : this might be due to uncertainties in the newly investigated experiments for which the material composition is not very well-known (« old » experiments) or also because, in these experiments, the fundamental mode was not completely established. Another explanation might be that the calculational models used in this study (cylindrical geometry with white boundary conditions) must be improved using mmore accurate self-shielding and collision probability (exact 2D) methods. However, if we consider only the experiments analyzed in the study performed at CEA in 1993, the new evaluation reduces the experiment/calculation discrepancies.

In order to clarify these questions, a selection from among the tested experiments must be made in order to define a set of experiments with which the benchmarking exercices can be performed with a very high level of confidence.

Furthermore, additional investigations must be performed, especially using reference codes such as a MONTE-CARLO code, in order determine a reference calculational scheme involving APOLLO-2.

TABLE I

Experiments Analyzed.

Experiment	*Country*	*Characte-ristic*	*Number of Keff*
ZPR	USA	UO_2 of several % of ^{235}U- Stainless Steel clad. several moderation ratios	6
CRISTO	France	UO_2, Zr clad. square Undermoderated and over moderated cores	2
VVER	Hungary	UO_2 of several % of ^{235}U, Zr clad - Hex. pitch -several moderation ratios and temperature	15
DIMPLE	England	UO_2 - 3% - Mod ratio =1. Square Al Clad.	1
EPICURE	France	UO_2 - 3.7% - MR = 1.2 - Zr clad ; Square	1
MELODIE	France	UO_2 - 3% - MR = 1.2 - Zr clad ; Square	1
AZUR	France	U Metal ; plates	3
CAMELEON	France	UO_2 - 3.25% - MR = 1.8 - Al clad ; Square	1
BNL	USA	UO_2 - 3% - Zr clad ; Square	5
TRX	USA	U metal - Hex. pitch	2
KRITZ	Sweden	UO_2 - square - Al clad.	1
BAPL	USA	UO_2 - square	3
H_2O exp.	USA	U metal - D_2O	5
D_2O exp.	USA	UO_2 - D_2O moderator	4
MIT (D_2O)	USA	UO_2 - D_2O moderator	3
ORNL	USA	Spherical Uranyl.	2

TABLE II :
Discrepancies in reactivity obtained with
JEF2.2 and the LEAL/DERRIEN evaluations (C-E in pcm)

Experiment	U235 JEF2.2		U235 Leal-Derrien		LD-JEF2.2
	Sl dens. at 4 eV	*(1-keff) / keff*	*Sl dens. at 4 eV*	*(1-keff) / keff*	
ZPRHiC-11	0.3578	136.00	0.3563	871.94	735.94
CRISTO 3	0.3641	348.00	0.3627	1077.49	729.49
V1103600130	0.4238	1930.77	0.4227	2520.68	589.90
V1103600080	0.4301	1636.86	0.4290	2207.16	570.30
ZPRHiC-9	0.4359	453.00	0.4349	985.11	532.11
V1103600020	0.4385	491.10	0.4395	1044.70	553.60
V1103610020	0.4407	1105.28	0.4395	1664.14	558.86
ZPRBo-2	0.4504	-136.00	0.4487	450.32	586.32
ZPRHiC-8	0.4651	839.00	0.4643	1296.29	457.29
ZPRBo-1	0.4852	-294.00	0.4842	184.34	478.34
V1274400020	0.4890	288.63	0.4881	716.90	428.27
DIMPLE	0.4929	32.00	0.4920	481.31	449.31
V1274406020	0.4970	-399.99	0.4961	26.21	426.20
H-MEM	0.5021	-235.00	0.5013	145.00	380.00
UH1.2	0.5049	-324.00	0.5040	121.15	445.15
V1273600130	0.5056	333.71	0.5049	727.05	393.34
ZPRHiC-6	0.5097	364.00	0.5087	837.05	473.05
V1273600080	0.5102	207.33	0.5095	587.23	379.90
V1273600020	0.5186	-979.51	0.5178	-609.96	369.55
H-UO61	0.5395	1174.00	0.5389	1369.50	195.50
V1273640130	0.5418	160.26	0.5410	561.23	400.98
MELODIE-1	0.5450	1129.00	0.5440	1588.85	459.85
V1273640080	0.5477	-92.81	0.5469	291.35	384.16
V1504400020	0.5491	339.55	0.5485	639.16	299.61
V1274472020	0.5513	-1451.52	0.5503	-1017.34	434.18
V1273640020	0.5514	-185.46	0.5506	190.56	376.02
V1273658130	0.5566	330.29	0.5558	737.19	406.91
H-OX33	0.5597	56.00	0.5589	399.59	343.59
V1273658080	0.5651	-347.89	0.5642	39.62	387.50
AZUR-834	0.5660	662.00	0.5651	1047.15	385.15
V1273658020	0.5694	-504.24	0.5685	-126.51	377.73
CAMELEON	0.5720	-939.00	0.5713	-592.07	346.93
V1503600020	0.5776	-304.09	0.5771	-47.38	256.71
AZUR-1031	0.5786	604.00	0.5777	989.70	385.70
H-OX44	0.5792	120.00	0.5786	426.81	306.81
BNLOX-13	0.5811	-575.00	0.5803	-217.90	357.10
V1273672020	0.5837	-821.10	0.5829	-443.33	377.78
AZUR-1249	0.5925	540.00	0.5916	926.51	386.51
BNLOX-16	0.6072	-323.00	0.6065	-18.40	304.60
TRX-1	0.6219	-145.00	0.6215	62.00	207.00
H-UO75	0.6281	1065.00	0.6278	1244.19	179.19
V1271600020	0.6287	942.81	0.6285	1114.59	171.78
H-OX37	0.6319	303.00	0.6314	539.90	236.90
BNLOX-20	0.6392	-266.00	0.6387	-17.10	248.90
KRITZ-20	0.6477	-120.00	0.6473	53.83	173.83
BAPL-1	0.6481	-149.00	0.6477	27.21	176.21

TABLE II (Continued) :

Discrepancies in reactivity obtained with
JEF2.2 and the LEAL/DERRIEN evaluations (C-E in pcm)

	U235 JEF2.2		*U235 Leal-Derrien*		
Experiment	*St. dens. at 4 eV*	*(1-keff) / keff*	*St. dens. at 4 eV*	*(1-keff) / keff*	*LD-JEF2.2*
V1503640020	0.6543	-1226.37	0.6538	-978.92	247.45
V1271618020	0.6642	1116.02	0.6638	1304.60	188.58
BAPL-2	0.6810	-179.00	0.6807	-37.59	141.41
BNLOX-29	0.6848	-520.00	0.6844	-331.60	188.40
H-UO87	0.6973	887.00	0.6971	1003.98	116.98
TRX-2	0.7098	-77.00	0.7089	42.00	119.00
V1501600020	0.7175	-85.03	0.7172	22.81	107.83
BAPL-3	0.7304	-209.00	0.7302	-110.48	98.52
BNLOX-41	0.7406	-232.00	0.7402	-101.30	130.70
D-UN8	0.7623	-64.00	0.7619	-89.00	-25.00
D-UN0	0.7705	-58.00	0.7702	-12.00	46.00
MIT-1	0.7715	69.00	0.7712	122.00	53.00
MIT-2	0.7934	280.00	0.7929	264.00	-16.00
MIT-3	0.8215	243.00	0.8207	255.00	12.00
ORNL-1	0.8302	329.00	0.8300	520.60	191.60
D-UN3	0.8399	-81.00	0.8395	-85.00	-4.00
D-UN5	0.8740	-7.00	0.8736	-41.00	-34.00
CRISTO 1	0.8960	-511.00	0.8956	-414.18	96.82
ORNL-10	0.9262	180.00	0.9261	300.90	120.90

	JEF2.2	Leal-Derrien
Average	105.44	411.35
St. deviation	624.21	678.60

TABLE III

Discrepancies in reactivity obtained with JEF2.2 and the LEAL/DERRIEN evaluations for experiments tested in 1993 at CEA (C-E in pcm)

	U235 JEF2.2		*U235 Leal-Derrien*		
Experiment	*St. dens. at 4 eV*	*(1-keff) / keff*	*St. dens. at 4 eV*	*(1-keff) / keff*	*LD-JEF2.2*
DIMPLE	0.4929	32.00	0.4920	481.31	449.31
UH1.2	0.5049	-324.00	0.5040	121.15	445.15
V1273600130	0.5056	333.71	0.5049	727.05	393.34
V1273600080	0.5102	207.33	0.5095	587.23	379.90
V1273600020	0.5186	-979.51	0.5178	-609.96	369.55
CAMELEON	0.5720	-939.00	0.5713	-592.07	346.93
V1503600020	0.5776	-304.09	0.5771	-47.38	256.71
BNLOX-13	0.5811	-575.00	0.5803	-217.90	357.10
TRX-1	0.6219	-145.00	0.6215	62.00	207.00
BNLOX-29	0.6848	-520.00	0.6844	-331.60	188.40
TRX-2	0.7098	-77.00	0.7089	42.00	119.00
BNLOX-41	0.7406	-232.00	0.7402	-101.30	130.70
ORNL-1	0.8302	329.00	0.8300	520.60	191.60

	JEF2.2	LEAL/DER.
Average	-245	47
St. deviation	428	400

Figure 1

Differences between the ^{235}U total cross-sections in the JEF2.2 and LEAL/DERRIEN evaluations. (LEAL/DERRIEN - JEF2.2)/JEF2.2 in %

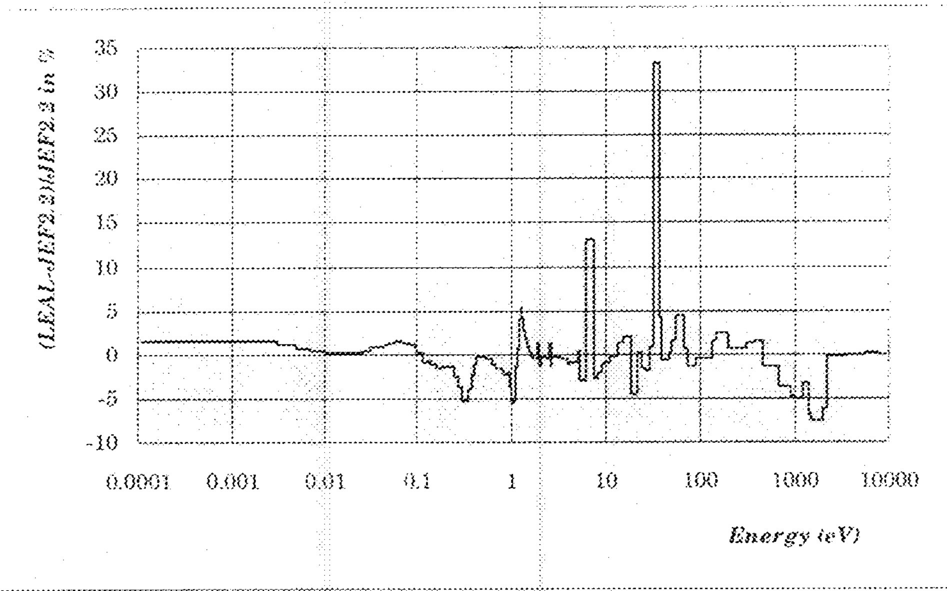

Figure 2

Differences between the ^{235}U elastic scattering cross-sections in the JEF2.2 and LEAL/DERRIEN evaluations. (LEAL/DERRIEN - JEF2.2)/JEF2.2 in %

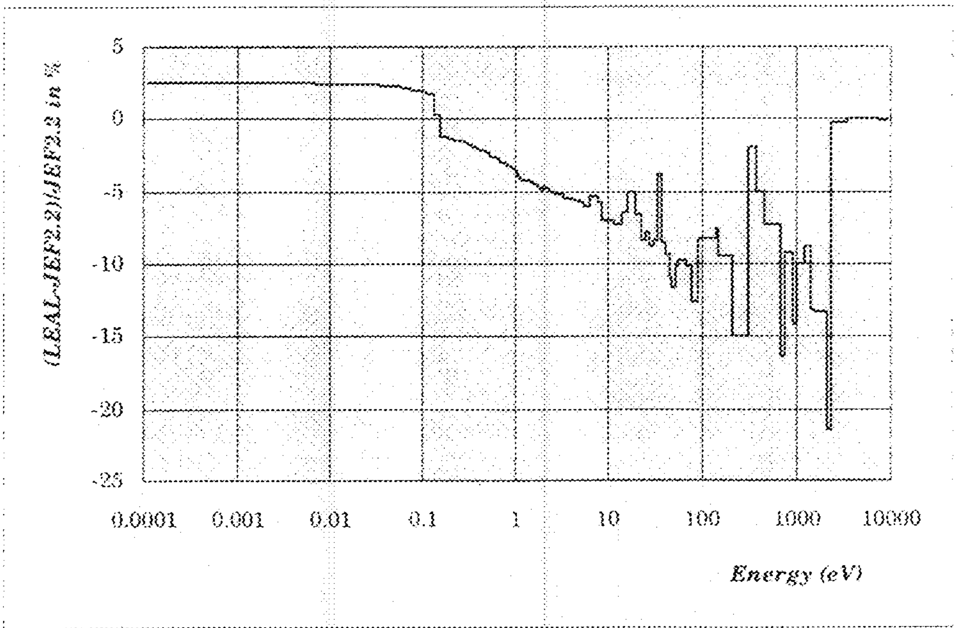

Figure 3

Differences between the ^{235}U fission cross-sections in the JEF2.2 and LEAL / DERRIEN evaluations. (LEAL / DERRIEN - JEF2.2) / JEF2.2 in %

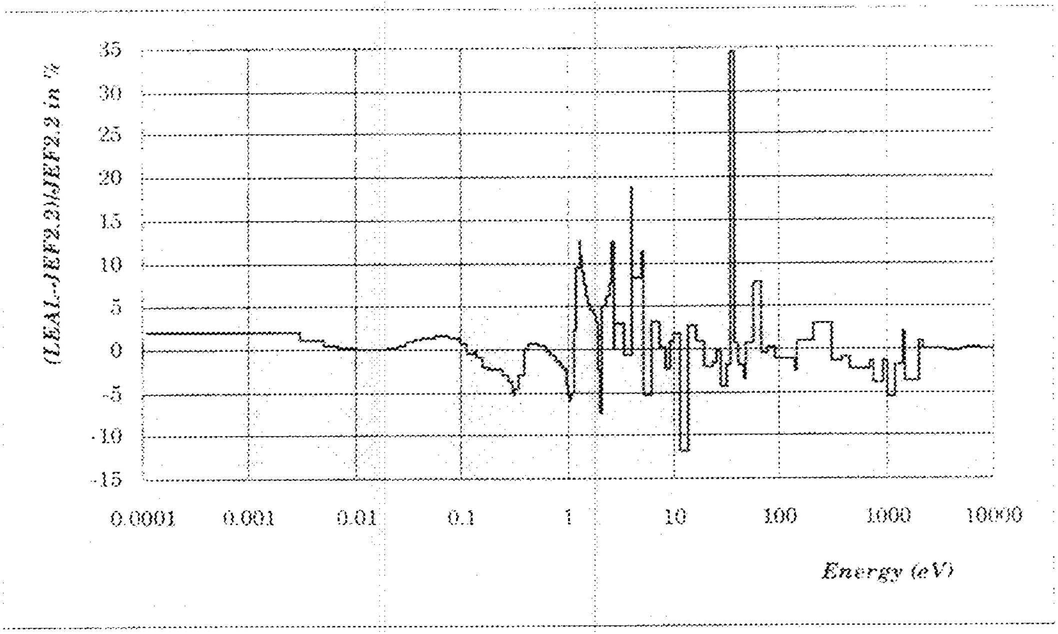

Figure 4

Differences between the ^{235}U capture cross-sections in the JEF2.2 and LEAL / DERRIEN evaluations. (LEAL / DERRIEN - JEF2.2) / JEF2.2 in %

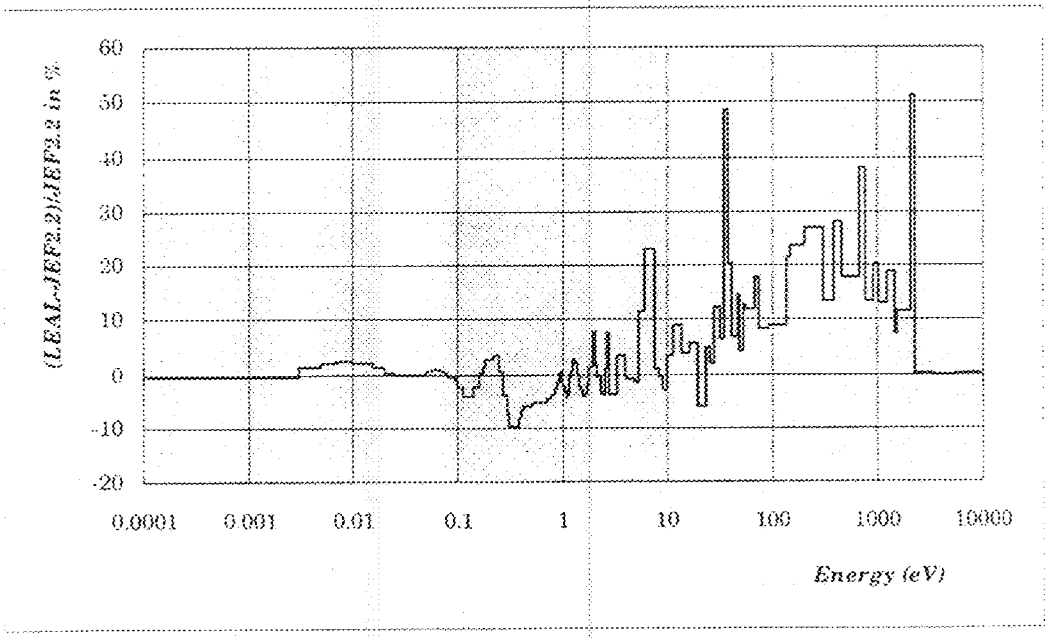

Figure 5

Differences between the ^{235}U fission / capture ratio in the JEF2.2 and LEAL / DERRIEN evaluations. (LEAL / DERRIEN - JEF2.2) / JEF2.2 in %

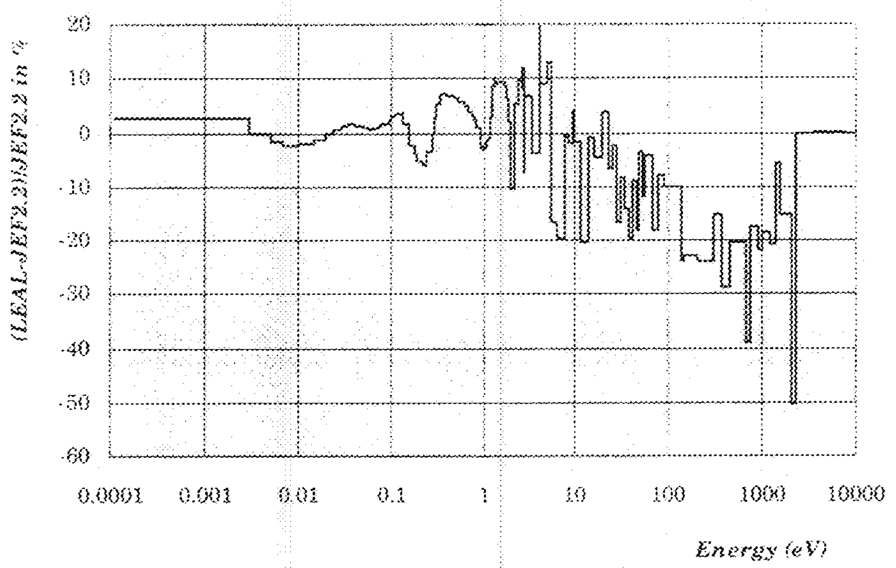

Figure 6

Differences between JEF2.2 and LEAL / DERRIEN evaluations for C-E on Keff
$\Delta\rho$ = *[LEAL / DERRIEN - JEF2.2] / LD×JEF2.2 in pcm.*

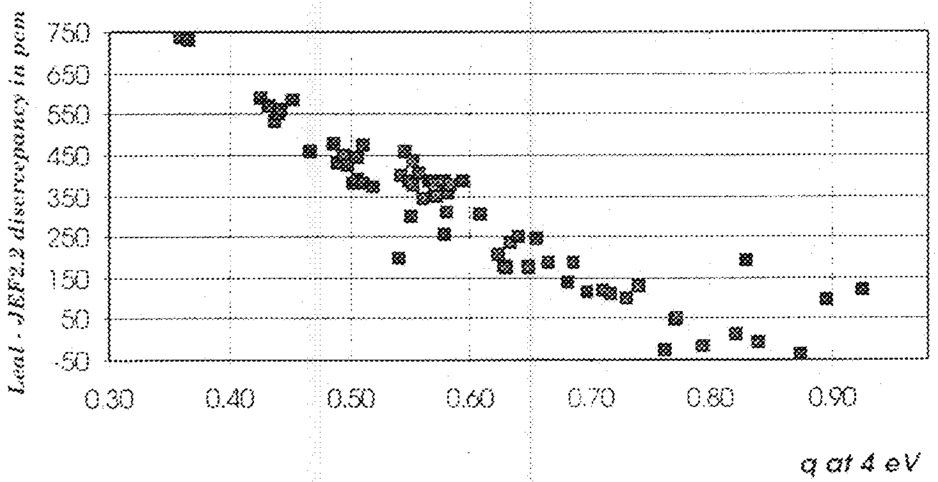

Figure 7
Differences in sensitivity profile for TRX2 experiment between LEAL/DERRIEN and JEF2.2 evaluations