

**Analysis, processing and integral testing
of the ^{235}U Leal-Derrien-Larson's evaluation.**

Keywords : JEFF3, U235, average resonance parameters, integral testing, Apollo2

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CONTENTS

I. Introduction	3
II. Basic comparisons.....	3
II-1 Average resonance parameter comparison in resolved range.....	3
II-2 Overview of JEF2.2 and LDL evaluations	6
III. Experimental validations	9
III-1 Westcott factors	9
III-2 Critical experiment UO ₂ /D ₂ O-H ₂ O.....	11
III-3 Isotopic evolution in PWR assembly	16
IV- Conclusions.....	16
V-ANNEXE.....	17

list of figures

Figure 1 Fission cross section for JEF2.2 and LDL evaluations	7
Figure 2 Capture cross section for JEF2.2 and LDL evaluations.....	7
Figure 3 Capture to fission ratio between 0.5 and 2250 eV.....	8
Figure 4 Capture Westcott factor.....	9
Figure 5 Fission Westcott factor.	10
Figure 6 keff SSCR2 versus δ_{25}	14
Figure 7 keff SSCR4 versus δ_{25}	15

list of tables

Table 1 $\langle \Gamma_f \rangle$ U235 $J^\pi = 3^-$	4
Table 2 $\langle \Gamma_f \rangle$ U235 $J^\pi = 3^-$	4
Table 3 $\langle \Gamma_f \rangle$ U235 $J^\pi = 4^-$	5
Table 4 $\langle \Gamma_f \rangle$ U235 $J^\pi = 4^-$	5
Table 5 Thermal values and resonance integrals in the resolved range 0.5-2.25 keV	6
Table 6 keff for 2.46% fuel and for 4% fuel	11
Table 7 δ_{25} SSCR2.....	12
Table 8 ρ_{28} SSCR2	12
Table 9 δ_{25} SSCR4.....	13
Table 10 ρ_{28} SSCR4	13
Table 11 U235 LDL $J^\pi = 3^-$	17
Table 12 U235 JEF2.2 $J^\pi = 3^-$	17
Table 13 U235 LDL $J^\pi = 4^-$	18
Table 14 U235 JEF2.2 $J^\pi = 4^-$	18
Table 15 U235 Leal-Derrien 1996 $J^\pi = 3^-$	19
Table 16 U235 Leal-Derrien 1996 $J^\pi = 4^-$	19
Table 17 U235 Leal-Derrien-Moxon 1997 $J^\pi = 3^-$	20
Table 18 U235 Leal-Derrien-Moxon 1997 $J^\pi = 4^-$	20

I. Introduction

The need of a new evaluation of ^{235}U arose from the discrepancies encountered analysis of spent fuel in power reactors and also in highly epithermal lattices when using JEF2.2 evaluation. The isotopic ratio $^{236}\text{U} / ^{238}\text{U}$ in spent fuels was consistently underestimate by few per cent. In highly epithermal lattices, the mean multiplication factor can be overestimate by 0.5% to 1% depending of the ^{235}U enrichment.

The Leal-Derrien-Larson's evaluation^[1] issued in august 1997 (later called LDL) was compared to JEF2.2 considering the calculations of the average resonance parameters : the level spacing, the reduced neutron width, the radiative width and the fission width and also the strength function.

Some comparisons on ponctual cross-sections of capture and fission calculated by NJOY94.66 nuclear data processing code will be shown. We give some figures concerning thermal values and resonance integrals.

Finally, we will conclude with integral testing using different kind of experiment : fission Westcott factor measured in a wide temperature range from 77 K (liquid nitrogen) to 600 K, critical experiments in the Spectral Shift Control Reactor which uses a mixture of heavy and light water to vary greatly the neutron spectrum from thermal to highly epithermal spectra, isotopic evolution in PWR assembly.

II. Basic comparisons

II-1 Average resonance parameter comparison in resolved range

Using the resonances file (ENDF code {MF=2, MT=151}) for each evaluation, we performed the averages discarding the fictitious levels outside the energy range 0-2.25 keV. For a given spin and parity of a level of the compound nucleus, the resonance parameters are the following : energy, neutron width, radiative width, and two fission widths. For the last ones, the absolute values are summed. The average values are given for each spin et parity of compound state within band energy of 450 eV. We give now the results for four evaluations in tables 1 to 4 for $J^\pi = 3^-$ or 4^- .

upper boundary	JEF2.2	LDL	LD96	LDM97	LD96/JEF2.2	LDM97/ JEF2.2	LDL/JEF2.2
450	37,52	42,21	48,82	40,28	1,30	1,07	1,13
900	43,00	46,28	50,19	45,13	1,17	1,05	1,08
1350	42,08	45,11	47,75	47,75	1,13	1,13	1,07
1800	38,56	41,76	42,43	42,43	1,10	1,10	1,08
2246	35,17	39,99	48,03	48,03	1,37	1,37	1,14
all	39,02	42,92	47,58	44,69	1,22	1,15	1,14

Table 1 $\langle \Gamma_r \rangle$ U235 $J^{\pi} = 3^-$.

upper boundary	JEF2.2	LDL	LD96	LDM97	LD96/JEF2.2	LDM97/ JEF2.2	LDL/JEF2.2
450	244,25	247,2	254,04	248,210	1,04	1,02	1,01
900	167,48	160,97	167,24	164,98	1,00	0,99	0,96
1350	125,94	122,66	120,78	120,78	0,96	0,96	0,97
1800	81,04	92,99	90,51	90,51	1,12	1,12	1,15
2246	62,99	70,29	72,02	72,02	1,14	1,14	1,12
all	137,12	142,42	143,50	141,75	1,05	1,03	1,04

Table 2 $\langle \Gamma_f \rangle$ U235 $J^{\pi} = 3^-$.

LDL : last evaluation of Leal-Derrien-Larson issued in august 1997

LD96 : Leal-Derrien issued in 1996

LDM97 : Leal-Derrien-Moxon issued in march 1997

upper boundary	JEF2.2	LDL	LD96	LDM97	LD96/JEF2.2	LDM97/JEF2.2	LDL/JEF2.2
450	37,19	42,16	48,82	40,18	1,31	1,08	1,13
900	44,08	46,19	50,19	45,31	1,14	1,03	1,05
1350	44,34	46,87	47,75	49,06	1,08	1,11	1,06
1800	38,62	44,00	42,43	44,68	1,10	1,16	1,14
2246	35,03	40,27	48,03	48,97	1,37	1,40	1,15
all	39,53	43,65	47,58	45,08	1,20	1,14	1,10

Table 3 $\langle \Gamma_r \rangle$ U235 $J^* = 4^-$.

upper boundary	JEF2.2	LDL	LD96	LDM97	LD96/JEF2.2	LDM97/JEF2.2	LDL/JEF2.2
450	208,22	223,85	226,50	224,55	1,09	1,08	1,08
900	173,57	170,57	174,01	174,15	1,00	1,00	0,98
1350	117,86	111,53	108,99	108,99	0,92	0,92	0,95
1800	85,01	97,701	95,13	95,13	1,12	1,12	1,15
2246	66,55	69,22	70,55	70,55	1,06	1,06	1,04
all	136,39	144,97	145,36	144,83	1,07	1,06	1,06

Table 4 $\langle \Gamma_r \rangle$ U235 $J^* = 4^-$.

LDL : last evaluation of Leal-Derrien-Larson issued in august 1997

LD96 : Leal-Derrien issued in 1996

LDM97 : Leal-Derrien-Moxon issued in march 1997

II-2 Overview of JEF2.2 and LDL evaluations

We show the thermal values at 2200 m/s for these two evaluations. They are close together except for fission cross-section where the values differ by 0.4%. The resonance integrals for fission and capture (infinite dilution) are given in table 5. We can see the differences are significant. In particular, the capture to fission ratio is lower by 7% in LDL evaluation.

evaluation	$\sigma_{n,\gamma}$	$\sigma_{n,f}$	v_t	η	I_f	I_c	I_c / I_f
JEF2.2	98.85	582.62	2.4374	2.08385	260,43	128,21	0,492
LDL	98.69	585.03	2.4367	2.08497	257,69	136,07	0,528

Table 5 Thermal values and resonance integrals in the resolved range 0.5-2.25 keV

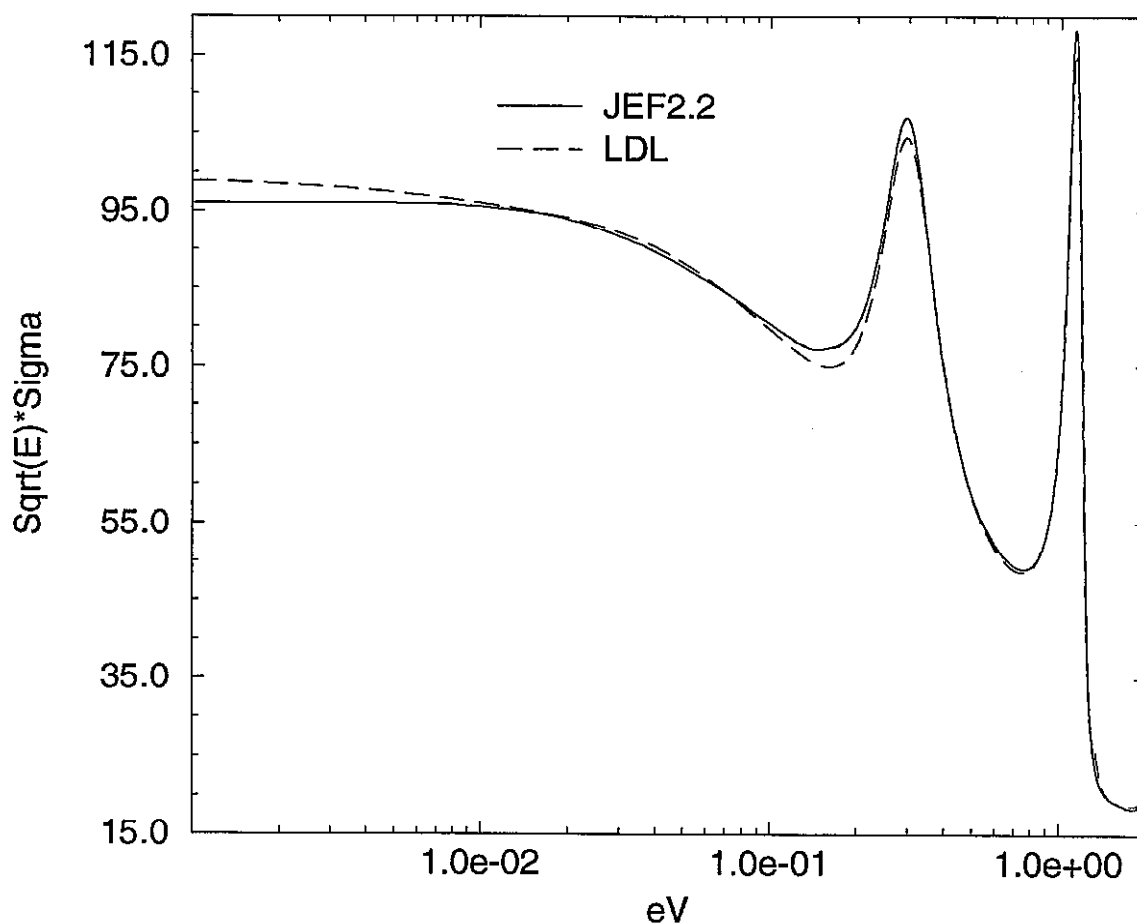


Figure 1 Fission cross section for JEF2.2 and LDL evaluations

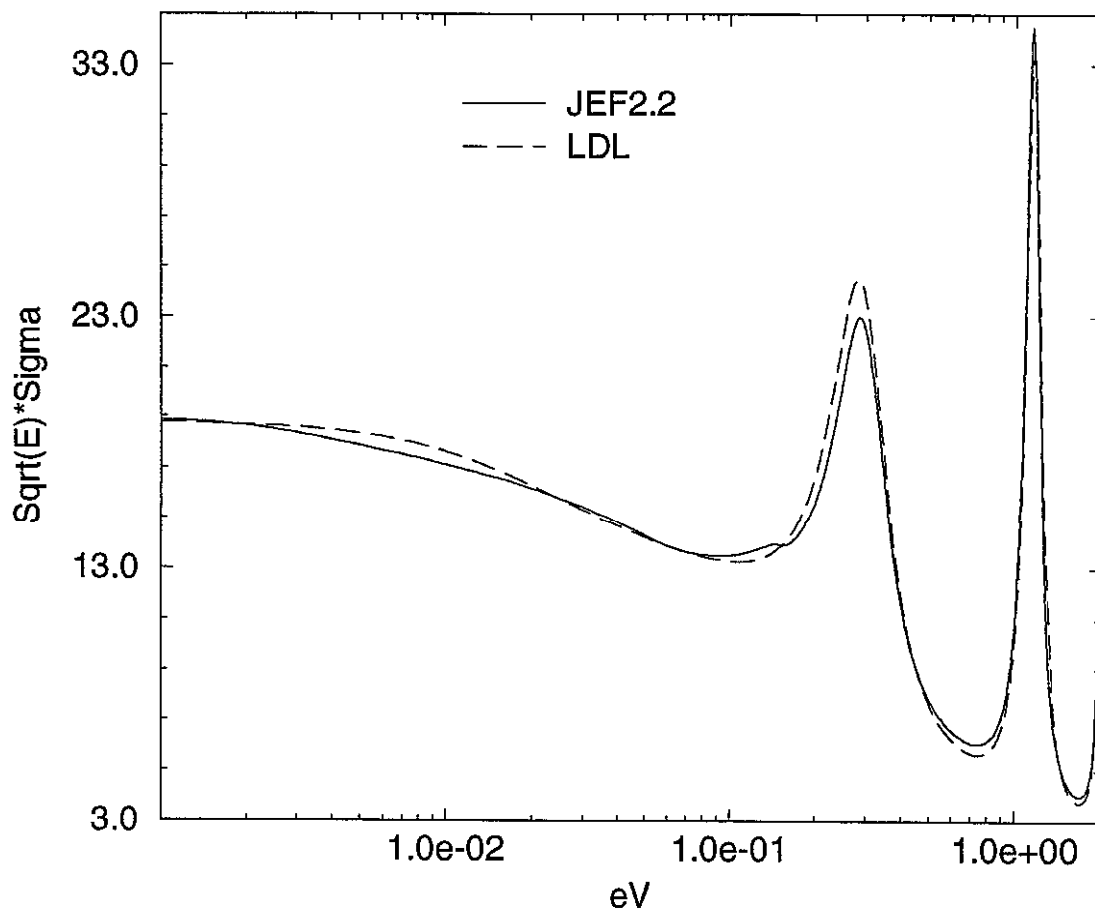


Figure 2 Capture cross section for JEF2.2 and LDL evaluations

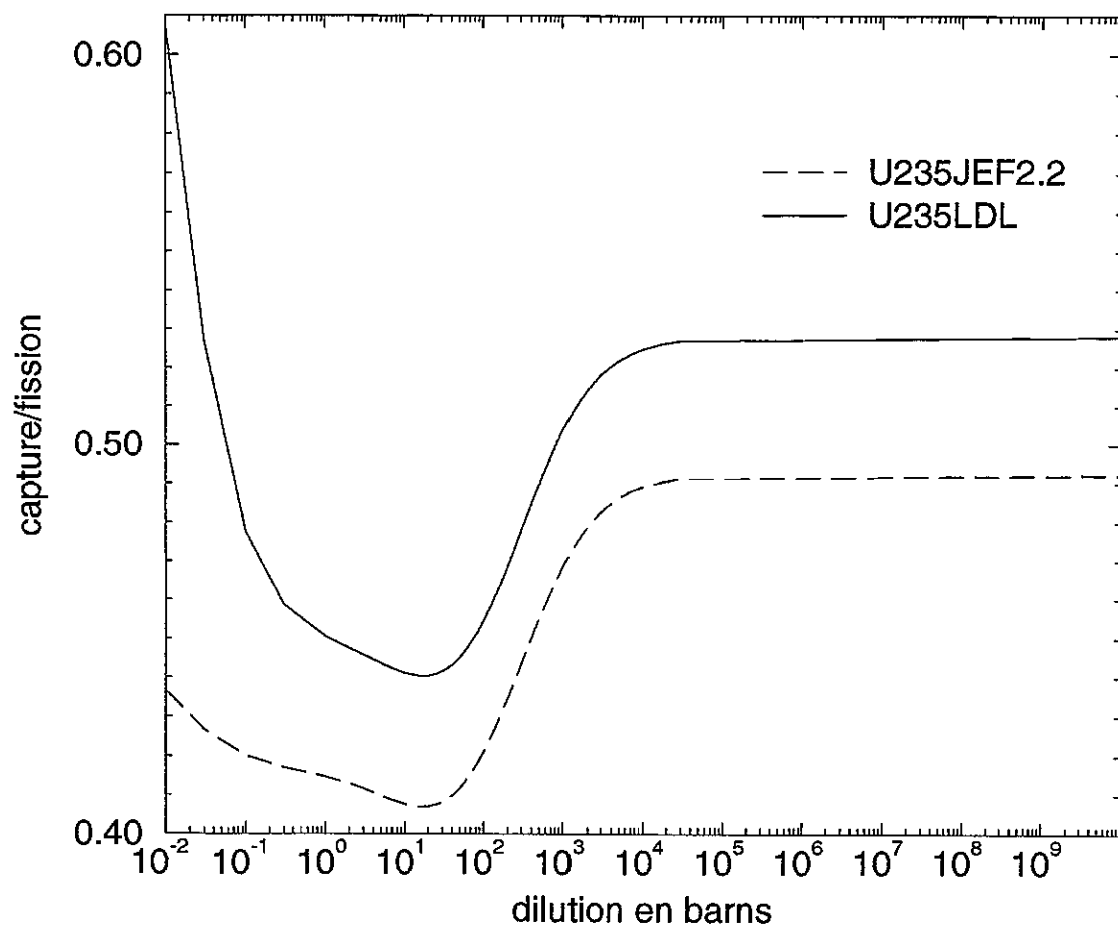


Figure 3 Capture to fission ratio between 0.5 and 2250 eV

III. Experimental validations

III-1 Westcott factors

The Westcott factors are useful to check the shape of the cross-section in the thermal range. The fission Westcott factor was measured in the Canadian heavy water reactor ZED-2^[2] with temperatures ranging from 77 K (liquid nitrogen) to 600 K. For fission cross section, the two evaluations give an equal agreement with experiment and are both within the experimental uncertainties. For capture cross-section, we only compare the calculated values of the Westcott factor (fig. 1), they show a good agreement on shape except for the highest temperatures where the LDL evaluation gives a lower decreasing slope with temperature.

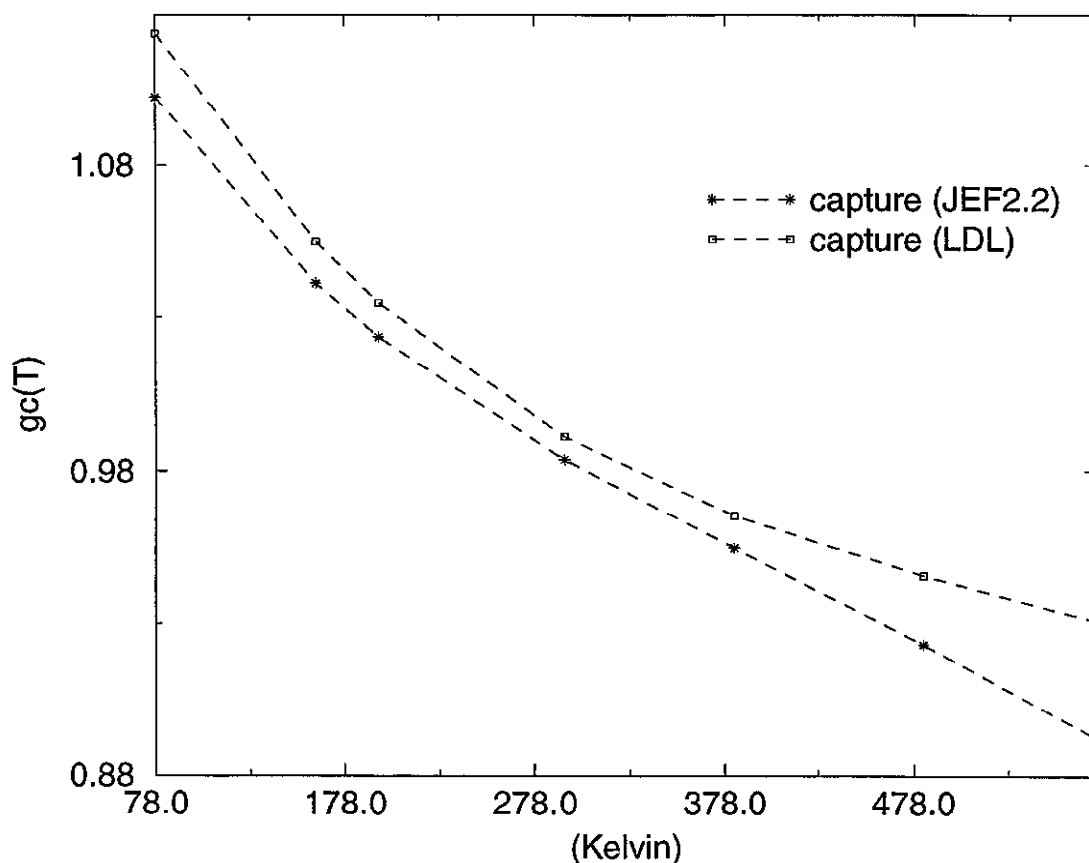


Figure 4 Capture Westcott factor

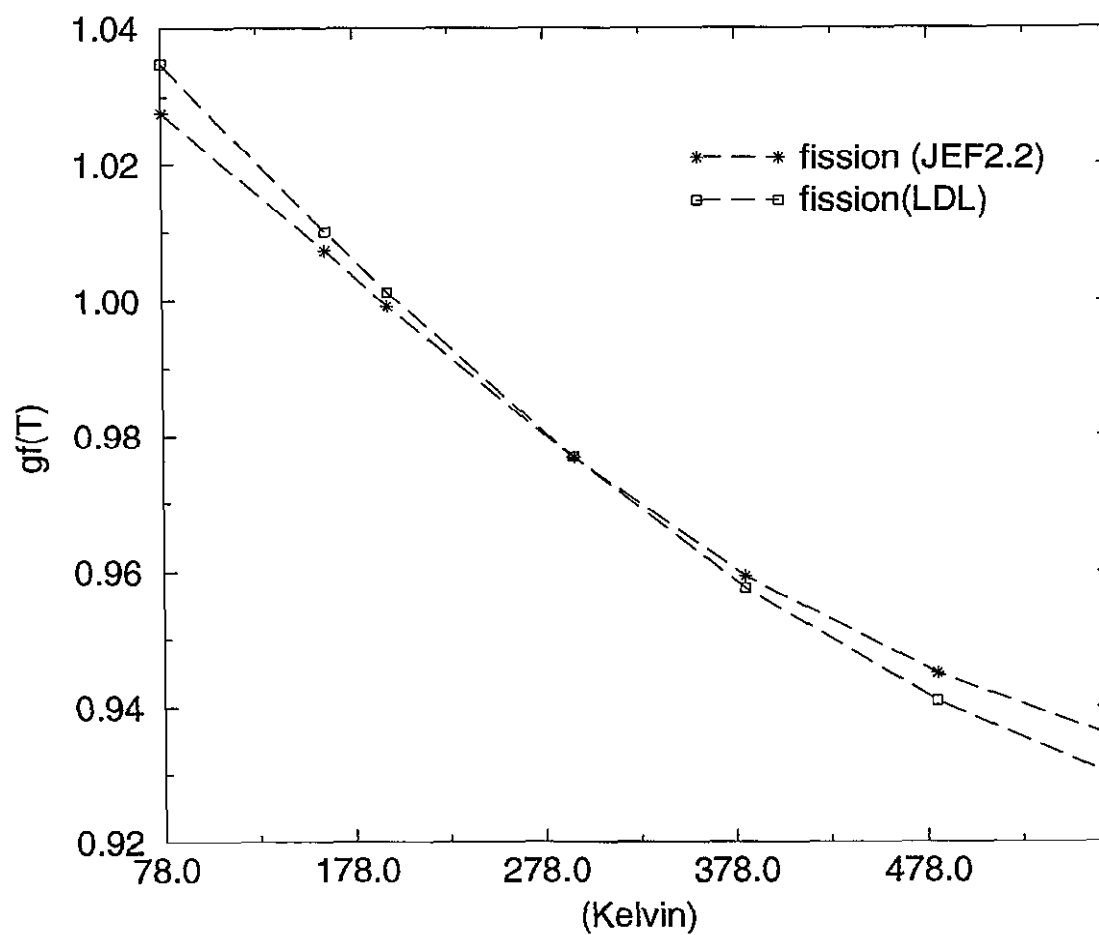


Figure 5 Fission Westcott factor.

III-2 Critical experiment UO₂/D₂O-H₂O

We study here a group of critical experiments made in the Spectral Shift Control Reactor^[3] where the spectrum can be shifted by varying the molar proportion of heavy water in light water. This experiment permits to highlight potential deficiencies in epithermal cross section. The analysis was conducted with Apollo2 code and its library CEA93V3 with 172 energy groups. We performed the analysis of 12 lattices with 4% ²³⁵U enrichment and 8 lattices with 2.46% ²³⁵U enrichment. We employed cylindrical core description calculated with Sn method (P1S16). The summarised of the keff results are given in table 10 but we have also results on spectral indices δ_{25} and ρ_{28} .

Core number	2.46% fuel		4% fuel	
	keff (JEF2.2)	keff (LDL)	keff (JEF2.2)	keff (LDL)
1	0,99941	0,99634	1,00018	0,99548
2	0,99797	0,99178	0,99972	0,99382
3	0,99863	0,99397	1,00827	0,99835
4	1,00233	0,99565	1,00858	0,99927
5	1,00259	0,99709	1,01231	1,00266
6	1,00322	0,99948	1,00842	0,99978
7	1,00806	1,00113	1,00932	0,99978
8	1,00001	0,99561	1,00724	0,99912
9			1,00514	0,99835
10			0,99829	0,99301
11			1,00694	0,99712
12			1,00377	0,99624
mean	1,00153	0,99638	1,00568	0,99775
dispersion	0.00306	0.00276	0.00416	0.00263

Table 6 keff for 2.46% fuel and for 4% fuel

Core number	$\delta_{25}(\text{exp})$	$\sigma(\delta_{25}(\text{exp}))$	$\delta_{25}(\text{JEF2.2})$	$\delta_{25}(\text{LDL})$	$(\text{C-E})/\sigma$ (JEF2.2)	$(\text{C-E})/\sigma$ (LDL)
1	0,151	0,001	0,149	0,148	-2,000	-3,000
2	0,392	0,003	0,396	0,394	1,333	0,667
3	0,264	0,001	0,266	0,264	2,000	0,000
4			0,418	0,416		
5			0,295	0,294		
6			0,184	0,183		
7	0,398	0,006	0,393	0,391	-0,833	-1,167
8	0,253	0,001	0,249	0,248	-4,000	-5,000
mean					-0,70	-1,53

Table 7 δ_{25} SSCR2

Core number	$\rho_{28}(\text{exp})$	$\sigma(\rho_{28}(\text{exp}))$	$\rho_{28}(\text{JEF2.2})$	$\rho_{28}(\text{LDL})$	$(\text{C-E})/\sigma$ (JEF2.2)	$(\text{C-E})/\sigma$ (LDL)
1	2,28	0,03	2,390	2,391	3,667	3,700
2	5,95	0,07	6,076	6,073	1,800	1,757
3	4,00	0,05	4,147	4,146	2,940	2,920
4			6,399	6,395		
5			4,588	4,586		
6			2,929	2,930		
7	6,29	0,08	6,115	6,111	-2,187	-2,238
8	3,95	0,06	3,946	3,946	-0,067	-0,067
mean					0,91	0,76

Table 8 ρ_{28} SSCR2

Core number	$\delta_{25}(\text{exp})$	$\sigma(\delta_{25}(\text{exp}))$	$\delta_{25}(\text{JEF2.2})$	$\delta_{25}(\text{LDL})$	$(\text{C-E})/\sigma$ (JEF2.2)	$(\text{C-E})/\sigma$ (LDL)
1	0,253	0,006	0,260	0,259	1,167	1,000
2			0,342	0,341		
3	0,855	0,022	0,906	0,904	2,318	2,227
4			0,832	0,830		
5			0,831	0,829		
6	0,699	0,010	0,739	0,737	4,000	3,800
7	0,758	0,012	0,771	0,769	1,083	0,917
8	0,535	0,009	0,563	0,561	3,111	2,889
9	0,478	0,007	0,481	0,479	0,429	0,143
10	0,307	0,002	0,312	0,311	2,500	2,000
11	0,893	0,008	0,928	0,926	4,375	4,125
12	0,575	0,007	0,588	0,586	1,857	1,571
mean					2,316	2,075

Table 9 δ_{25} SSCR4

Core number	$\rho_{28}(\text{exp})$	$\sigma(\rho_{28}(\text{exp}))$	$\rho_{28}(\text{JEF2.2})$	$\rho_{28}(\text{LDL})$	$(\text{C-E})/\sigma$ (JEF2.2)	$(\text{C-E})/\sigma$ (LDL)
1	4,12	0,31	4,299	4,297	0,577	0,571
2			5,632	5,629		
3	15,4	0,7	14,580	14,563	-1,171	-1,196
4			13,393	13,379		
5			13,388	13,372		
6	11,2	0,5	11,910	11,894	1,420	1,388
7			12,425	12,410		
8			9,113	9,104		
9	8,13	0,06	7,815	7,807	-5,250	-5,383
10	5,08	0,10	5,111	5,125	0,310	0,450
11	14,9	0,20	14,875	14,860	-0,125	-0,200
12	9,80	0,29	9,458	9,448	-1,179	-1,214
mean					-0,774	-0,798

Table 10 ρ_{28} SSCR4

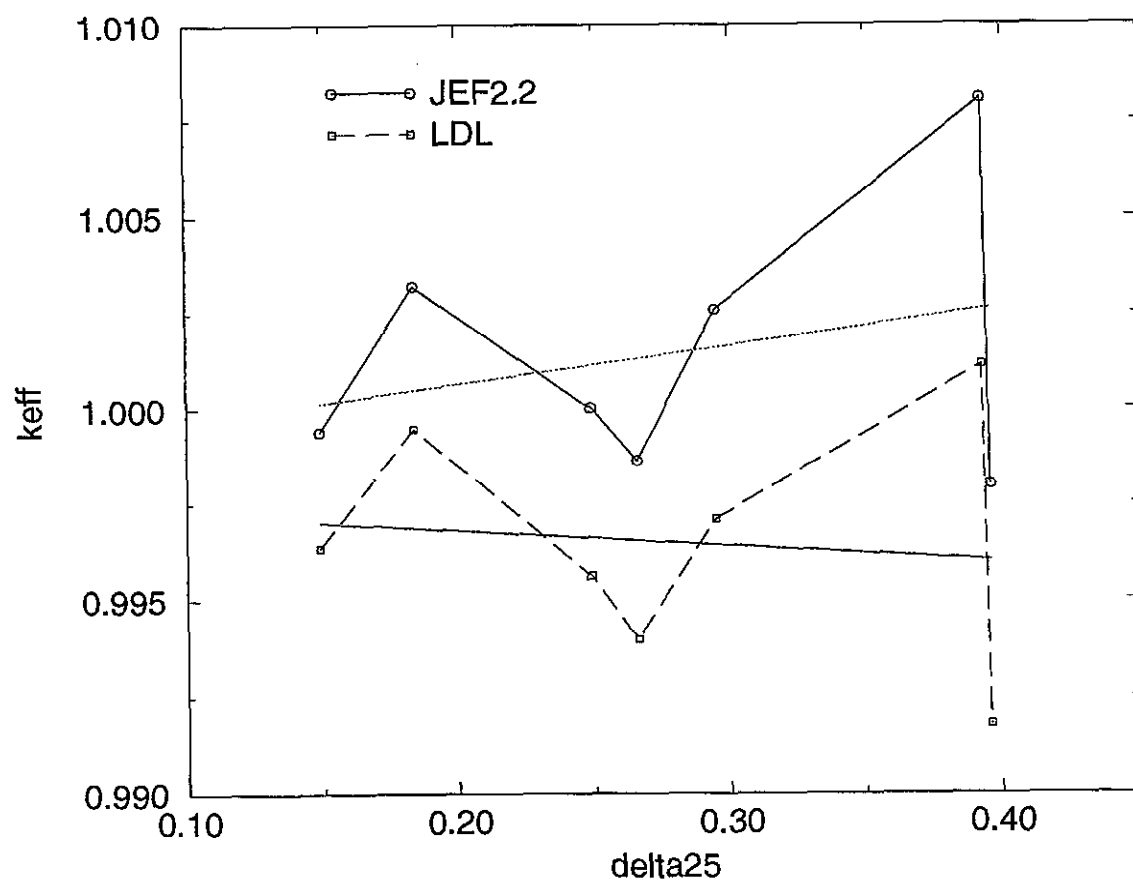


Figure 6 keff SSCR2 versus δ_{25} .

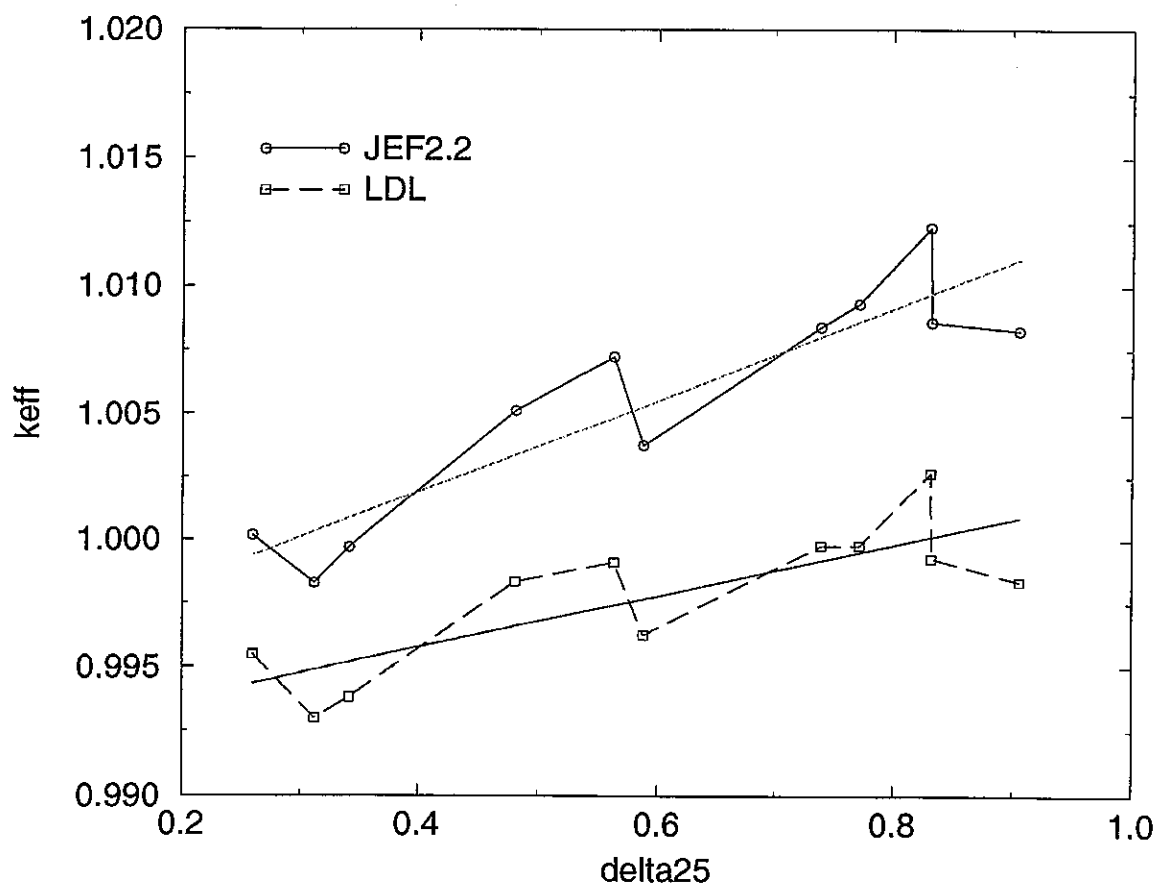


Figure 7 k_{eff} SSC4 versus δ_{25} .

III-3 Isotopic evolution in PWR assembly

We give a comparison on Uranium isotopic ratios calculated with Apollo2 code for a pin irradiated in PWR assembly of the EDF reactor Gravelines to a burnup of 27000 MWj/t. The main interesting conclusion is that the underestimation of the $^{236}\text{U}/^{238}\text{U}$ and $^{238}\text{Pu}/^{239}\text{Pu}$ ratios obtained with JEF2.2 evaluation is now reduced by 3% using the LDL's evaluation.

IV- Conclusions

The Leal-Derrien-Larson evaluation improves the agreement between calculation and experiment for lattices with epithermal spectra and high ^{235}U enrichment. The prediction of the ratio $^{236}\text{U}/^{238}\text{U}$ in spent fuel with this new evaluation is significantly improved compare to JEF2.2. The validation of this evaluation with experiment is still under study to give a definite conclusion but these first tests are interesting.

V-ANNEXE

E _{min}	E _{max}		$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle$ (10 ⁻³ eV)	$\langle \Gamma_\gamma \rangle$ (10 ⁻³ eV)	$\langle \Gamma_f \rangle$ (10 ⁻³ eV)	S _{0J} (10 ⁻⁴)
0.274	447.74	339	1.320	0.122	42.21	247.2	0.927
450.64	899.32	266	1.687	0.169	46.28	160.97	0.982
902.03	1349.51	260	1.721	0.181	45.11	122.66	1.054
1350.13	1798.93	249	1.802	0.187	41.76	92.99	1.037
1800.32	2246.14	319	1.398	0.150	39.99	70.29	1.071
0.274	2246.14	1433	1.568	0.159	42.92	142.42	1.014

Table 11 U235 LDL Jⁿ =3⁻.

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle$ (10 ⁻³ eV)	$\langle \Gamma_\gamma \rangle$ (10 ⁻³ eV)	$\langle \Gamma_f \rangle$ (10 ⁻³ eV)	S _{0J} (10 ⁻⁴)
0.277	447.71	309	1.448	0.130	37.52	244.25	0.896
450.74	899.	258	1.737	0.181	43.00	167.48	1.043
902.0	1349.7	260	1.722	0.185	42.08	125.94	1.072
1350.	1798.8	250	1.792	0.186	38.56	81.04	1.039
1800.3	2249.4	324	1.386	0.146	35.17	62.99	1.053
0.277	2249.4	1401	1.606	0.163	39.02	137.12	1.016

Table 12 U235 JEF2.2 Jⁿ =3⁻.

N : Number of resonances in range [E_{min},E_{max}]

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle (10^{-3} \text{eV})$	$\langle \Gamma_\gamma \rangle (10^{-3} \text{eV})$	$\langle \Gamma_f \rangle (10^{-3} \text{eV})$	S _{0f} (10 ⁻⁴)
0.000	449.94	505	0.891	0.093	42.16	223.85	1.047
451.43	899.83	322	1.393	0.156	46.19	170.57	1.119
901.06	1349.67	298	1.505	0.163	46.87	111.53	1.083
1350.55	1799.54	276	1.627	0.171	44.00	97.701	1.053
1801.28	2247.93	331	1.349	0.163	40.27	69.22	1.207
0.000	2247.93	1732	1.299	0.143	43.65	144.97	1.098

Table 13 U235 LDL Jⁿ =4-

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle (10^{-3} \text{eV})$	$\langle \Gamma_\gamma \rangle (10^{-3} \text{eV})$	$\langle \Gamma_f \rangle (10^{-3} \text{eV})$	S _{0f} (10 ⁻⁴)
1.136	449.78	444	1.010	0.101	37.19	208.22	1.001
451.61	899.8	299	1.499	0.171	44.08	173.57	1.141
900.97	1349.3	298	1.504	0.170	44.34	117.86	1.113
1350.3	1799.6	277	1.622	0.180	38.62	85.01	1.110
1801.9	2250.0	333	1.346	0.158	35.03	66.55	1.178
1.136	2250.0	1651	1.363	0.163	39.53	136.39	1.109

Table 14 U235 JEF2.2 Jⁿ =4

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle$ (10 ⁻³ eV)	$\langle \Gamma_r \rangle$ (10 ⁻³ eV)	$\langle \Gamma_f \rangle$ (10 ⁻³ eV)	S _{0f} (10 ⁻⁴)
.268	447.787	322	1.390	.121	48.82	254.04	.870
450.75	899.13	266	1.686	.178	50.19	167.24	1.057
902.06	1349.64	260	1.721	.180	47.75	120.78	1.044
1350.3	1798.92	249	1.802	.185	42.43	90.51	1.026
1800.28	2246.14	319	1.398	.153	48.03	72.02	1.097
.268	2246.14	1416	1.587	.161	47.58	143.50	1.014

Table 15 U235 Leal-Derrien 1996 Jⁿ =3

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle$ (10 ⁻³ eV)	$\langle \Gamma_r \rangle$ (10 ⁻³ eV)	$\langle \Gamma_f \rangle$ (10 ⁻³ eV)	S _{0f} (10 ⁻⁴)
.000	449.84	496	.907	0.095	46.94	226.50	1.045
451.31	899.87	322	1.393	.165	49.73	174.01	1.183
901.03	1349.52	298	1.505	.162	49.06	108.99	1.077
1350.53	1799.49	276	1.627	.172	44.68	95.13	1.057
1801.22	2247.93	331	1.350	.168	48.97	70.55	1.244
.000	2247.93	1723	1.305	.146	47.86	145.36	1.119

Table 16 U235 Leal-Derrien 1996 Jⁿ =4

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle (10^{-3} \text{eV})$	$\langle \Gamma_r \rangle (10^{-3} \text{eV})$	$\langle \Gamma_f \rangle (10^{-3} \text{eV})$	S _{0J} (10 ⁻⁴)
.294	447.787	322	1.390	.125	40.28	248.210	.897
450.73	899.13	266	1.686	.177	45.13	164.98	1.051
902.06	1349.64	260	1.721	.180	47.75	120.78	1.044
1350.2	1798.92	249	1.802	.185	42.43	90.51	1.026
1800.28	2246.14	319	1.398	.153	48.03	72.02	1.097
.268	2246.14	1416	1.587	.161	44.69	141.75	1.019

Table 17 U235 Leal-Derrien-Moxon 1997 J^π =3⁻

E _{min}	E _{max}	N	$\langle D \rangle$ (eV)	$\langle \Gamma_n^0 \rangle (10^{-3} \text{eV})$	$\langle \Gamma_r \rangle (10^{-3} \text{eV})$	$\langle \Gamma_f \rangle (10^{-3} \text{eV})$	S _{0J} (10 ⁻⁴)
.000	449.82	496	.907	.095	40.18	224.55	1.032
451.31	899.87	322	1.393	.165	45.31	174.15	1.186
901.03	1349.52	298	1.505	.162	49.06	108.99	1.077
1350.53	1799.49	276	1.627	.172	44.68	95.13	1.057
1801.22	2247.93	331	1.350	.168	48.97	70.55	1.244
.000	2247.93	1723	1.305	.146	45.08	144.83	1.119

Table 18 U235 Leal-Derrien-Moxon 1997 J^π =4⁻

^[1] L.C. Leal, H. Derrien, N.M. Larson and R.Q. Wright « R-matrix analysis of ²³⁵U neutron transmission and cross sections in energy range 0 eV to 2.25 keV. ORNL/TM report to be publish.

^[2] R.T. Jones and A.Okazaki, « Dependence of the effective cross sections on thermal neutron temperature, AECL-6483 (1979) ; « Measured dependence of some effective cross sections on thermal neutron temperatures in the range -195°C to 20°C », AECL-8844 (1985)

^[3] T.C. Englender et al, « Spectral shift control reactor, basic physics program, Measurement and analysis of uniform lattices of slightly enriched UO₂ moderated by D₂O-H₂O mixtures », BAW-1273 (1963)