

Contribution to the validation of the new ^{235}U evaluation

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ABSTRACT

This paper aims to contribute to the undergoing effort devoted to the validation of the new ^{235}U evaluation. The evaluation considered here is the one issued in early 1997 by Derrien et al.¹ from Oak-Ridge and referred in early JEF documents as Leal-Derrien-Larson evaluation. Since there was a previous evaluation issued by the same group at Oak Ridge (leal et al.²) we make the precision here that we are concerned with the last evaluation released by this group and which was adopted in the JEFF3.0 starter file, this is why we will refer here to the ^{235}U evaluation in JEFF3.0.

The effect of this new evaluation on the effective multiplication factor of various media was studied. The configurations investigated covers a wide range of applications, namely: uranium solutions (high and low enrichment), mixed uranium and plutonium solutions, dry powders of uranium dioxide and finally UO_2 lattices. Variable moderation ratios were considered in order to establish a trend with spectrum hardness. Calculations were made using the new criticality package CRISTAL with application libraries based on JEF2.2 except for ^{235}U for which both JEF2.2 and JEFF3.0 evaluations were used. The comparison of results obtained with these two evaluations showed negligible differences in the calculated k-effective for low enriched uranium solution and for mixed uranium and plutonium solutions, whereas significant discrepancies were observed for high enriched solutions, wet uranium dioxide powders and for UO_2 pins with a visible trend with spectrum hardness. The comparison with experimental values suggest that this new evaluation is performing better than the one in JEF2.2.

This paper investigated also the effect of ^{235}U data processing using two versions of NJOY (94.66 and 89.62). The difference being mainly in the multigroup fission spectrum generated. Results showed that this last effect is generally small except for highly enriched solutions with high uranium concentrations for which the effect can reach 500 to 600 pcm. This study helped to understand the discrepancies observed in the past³ between pointwise codes (MONK-7 and TRIPOLI-4) and multigroup ones (APOLLO2-MORET4). The multigroup application library for this last system was processed by NJOY-89.62 where an approximation in the GROUPN module results to fission spectra for fissile nuclides that is harder than the actual one.

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I. INTRODUCTION

Several studies indicated in the past the necessity of improving the ^{235}U evaluation used in JEF2.2 and ENDF/BVI-rev2. In particular, the adjustment procedure conducted by Cathalau et al.⁴ suggested an increase of about 10 to 13 % to the capture cross section in the resonance range. The thirteen experiments investigated by Cathalau et al. were mainly buckling measurements. Another experimental evidence that suggests a need for improvements in the ^{235}U capture cross section is the analysis of isotopic composition of irradiated fuels. In fact, typical discrepancy⁵ between calculations and measurements for the $^{236}\text{U}/^{238}\text{U}$ ratio is about $(-4.8 \pm 0.8) \%$. Lubitz⁶ proposed a modification to the ENDF/BVI-rev2 evaluation where he increased the capture width. His evaluation was included in ENDF/BVI-rev3. However, this evaluation was not considered as satisfactory since the high resolution measurements were not well reproduced by this evaluation. Leal et al.² from Oak Ridge proposed in 1995 a re evaluation of ^{235}U -resonance region up to 2250 eV. Studies with this evaluation showed significant differences in the calculation of integral parameters for intermediate systems compared to JEF2.2. For instance, Gagnier and Nouri⁷ found differences up to 1000 pcm in the calculated k_{eff} for uranium wet powder systems and for high-enriched uranium solutions at high concentrations. However prediction improvements were not general. In fact, considering the initial set of thirteen experiments, Cathalau and Blaise⁸ found in average a better agreement with experiments for this evaluation than for JEF2.2. Surprisingly, the situation was reversed when they considered a different set of experiments. These authors concluded to a need of careful selection of experiments and to the use of reference codes to establish the C/E. Rowlands⁹ made a proposal of benchmarks to be used for the validation of this evaluation. Nevertheless, this evaluation was not adopted in ENDF/BVI since there were outstanding questions principally related to Moxon's criticism¹. A new evaluation was issued in late '96 (or beginning '97) and was adopted in the JEFF3.0 starter file. C. Dean¹⁰ et al. made a comparison between the different ^{235}U evaluations using the set of experiments recommended by Rowlands. A part from few experiments (two in the intermediate energy range and a TRX configuration) the latest evaluation was found to perform very well. C. Mounier¹¹ also processed this last evaluation and first validations were presented at the last JEFF meeting by C. Mounier^{11,12} and by M-C. Alet et al¹³. These studies considered analysis of PWR irradiated fuels (GRAVELINES : 4.5 % initial enrichment irradiated during two cycles, BUGEY : initial 3.5 % uranium enrichment irradiated during 1.5, 2 or 3 cycles, SLB1 : MOX recycling with burnups of 30 and 45 GWd/t), as well as measurements of Westcott factor, and buckling for different UO_2 lattices. The most convincing results were those of irradiated fuel inventory (GRAVELINES where the discrepancy of $^{236}\text{U}/^{238}\text{U}$ ratio were reduced by about 3 % in absolute value and SLB1 where the discrepancies were reduced from -5 % or -6 % (JEF2.2) to 0.6 % or 1.6 % (JEFF3.0)). For buckling measurements important improvements were obtained for the CRISTO-3 configuration ($q = 0.3$) since the initial over-estimation with JEF2.2 (1.3 %) was reduced to 0.5 % with JEFF3.0 and for the Caméléon configuration (0.8 % discrepancy with JEF2.2 compared to 0.4 % with JEFF3.0). For the other configurations (CRISTO-1 and -2, Epicure UH1.2 and ZPR HiC6) the differences are rather small or the agreement between calculation and experiments are less good for JEFF3.0 than for JEF2.2 (CRISTO-2 for instance with -0.3 % with JEF2.2 and -0.5 % with JEFF3.0).

The aim of the present paper is to extend this validation. To this end a wide range of configurations (critical experiments) is considered with a variety of fuel compositions and spectra (uranium and mixed (U+Pu) solutions with various concentrations, wet UO_2 powders and uranium lattices with variable pitches). The calculations were performed using the new calculation package developed in France for criticality-safety studies which is presented in paragraph IV. The results of calculations are presented in paragraph V with a systematic comparison between the two evaluations in order to assess

the reactivity effects and a confrontation with experiments for demonstrating the accuracy prediction of the new JEFF3.0 evaluation compared to the one of JEF2.2. Another point is studied in the results sections i.e the influence of the processing (NJOY version) on the calculated k-effective. Finally, conclusions will summarise the different findings of this study.

II. CROSS SECTIONS COMPARISON

In this sections preliminary comparisons are presented between the studied ^{235}U evaluations. Table 1 gives the comparison of thermal sections and tables 2 and 3 give the resonance integrals in the resolved and unresolved resonance range (all these data were taken from reference 12). The differences in thermal data (2200 m/s) are very small (less than 0.2% decrease in the capture, 0.4% increase in the fission and negligible change in nu bar; the resulting eta values are quite similar). However, the comparison of the resonance region integrals in table 2 shows important increase of the capture cross section and decrease of fission (about 6% increase of the capture resonance integral and 1% decrease of the fission). No significant change is observed in the unresolved resonance range region which is may be a weakness in this evaluation as suggested by C. Dean¹⁰ and C. Mounier¹².

Evaluation	capture (barn)	fission (barn)	nu bar	eta
JEF2.2	98.85	582.62	2.4374	2.08385
JEFF3.0	98.69	585.03	2.4367	2.08497

Table 1: Comparison of ^{235}U thermal ($v = 2200$ m/s) data

Evaluation	capture (barn)	fission (barn)	alpha = capture/fission
JEF2.2	128.21	260.43	0.492
JEFF3.0	136.07	257.69	0.528

Table 2: Comparison of ^{235}U resolved resonance integrals

Evaluation	capture (barn)	fission (barn)	alpha = capture/fission
JEF2.2	2.9677	8.5449	0.347
JEFF3.0	2.9687	8.5435	0.347

Table 3: Comparison of ^{235}U unresolved resonance integrals

Figures 1 to 3 give the comparison of capture, fission cross sections and of eta (defined as $\eta = \frac{\nu\sigma_f}{\sigma_a}$).

For energies between 6 eV and 2250 eV the capture cross-section was substantially increased, the fission cross section was decreased and consequently the eta value was decreased. As expected, no change is visible in the unresolved energy range (above 2250 eV). For thermal energies, there are differences in peaks and in the valleys of the resonances.

III. INVESTIGATED EXPERIMENTS

The performance of the new evaluation is to be verified in a wide range of applications before adoption in application libraries. Our contribution emphasises configurations encountered in nuclear fuel cycle operations away from reactor. The experiments investigated belong to the five following categories: low enriched uranium solutions (LEU_SOL_THERM), high enriched uranium solutions (HEU_SOL_THERM), mixed uranium and plutonium solutions (MIX_SOL_THERM), powder of uranium dioxide of low enrichment, density and moderation (LEU_COMP_INTER) and finally arrays of low enriched uranium pins (LEU_COMP_THERM). The names between brackets correspond to the ICSBEP¹⁴ classification which was adopted here since the majority of the experiments were taken from this reference; the last part of the name is an indication of the spectrum in the system (thermal , intermediate or fast). Our study is not complete since there are at least two important categories missing (MIX_COMP_THERM : arrays of mixed uranium and plutonium pins) and HEU_MET_FAST (uranium metallic systems), calculations being in progress.

The following sub-sections give some more details on the experiments.

* LEU SOL THERM :

The first experiment in this category (LEU_SOL_THERM_001_01) was carried out at Los Alamos in a bare cylindrical tank (SHEBA) with a 5 % enriched uranium fluoride solution at a concentration of 980 g/l. The next three experiments (LEU_SOL_THERM_002_C01 to C03) were performed at Oak Ridge with a similar solution but with lower concentrations (from 450 g/l to 500 g/l). The other investigated experimental program involved bare spheres containing 10% enriched uranyl nitrate solutions with a concentration ranging from 170 g/l to about 300 g/l.

* MIX SOL THERM :

The experiments in this category were made in different cylindrical tanks with homogeneous mixed ($U_{\text{nat}} + \text{Pu}$) nitrate solutions. The uranium concentration range covered extends from 10 to 260 g(U)/l with a ratio of plutonium Pu/(U+Pu) of about 20, 30 and 50 %.

* HEU SOL THERM :

The first set of experiments was performed at Oak Ridge in water reflected spheres of 93 % enriched UO_2F_2 solutions (HEU_SOL_THERM_009 to HEU_SOL_THERM_012). The uranium concentration ranged from 20 g/l to approximately 700 g/l.

The HEU_SOL_THERM_013 and HEU_SOL_THERM_001 experiments were respectively carried out in unreflected spheres and cylinders with 93 % enriched $\text{UO}_2(\text{NO}_3)_2$ solutions. In the first ones, boron was added to the uranium solution.

The other experiments investigated involved a water reflected cylindrical tank of 89% enriched uranium nitrate solution with gadolinium.

For uranyl nitrate solutions, the concentration ranged from 20 g(U)/l to 400 g(U)/l.

These experiments involved arrays of low enriched UO_2 pins. The uranium enrichment varied from 2.6 % to 4.6 %. Different lattices of water moderated were considered: square and triangular lattices with pitches from 1.26 cm to 2.3 cm were calculated. Some of these configurations involved soluble poison (boron or gadolinium).

The eight investigated experiments are part of the experimental program MARACAS, performed in Valduc (France) in 1984. They involved two arrays of cans containing a low enriched uranium oxide powder with an H/U ratio of 2, 2.5 or 3, reflected by polyethylene.

IV. CALCULATION METHODS

For this study we used the new criticality-safety package CRISTAL (see figure 4). This package contains two calculation routes :

- * a multigroup scheme (the XMAS 172-group structure) using the assembly code APOLLO-2 and the Monte-Carlo code MORET-4. APOLLO-2 was used here for self-shielding calculations using the generalised Livolant-Jeanpierre Formalism and for flux calculations (Pij method) allowing, when appropriate, the homogenisation of the cell. MORET-4 uses homogenous cross sections generated by APOLLO-2 and a general Pn-like anisotropy representation. The standard application library CEA93-V3 derived from JEF2.2 and processed using NJOY-89.62 was used for all isotopes except for ^{235}U for which two other isotopes were processed by C. Mounier using NJOY-94.66 : one JEF2.2 isotope and the other from the JEFF3.0 evaluation.
- * a pointwise scheme using the Monte-Carlo code TRIPOLI-4 with application library derived from JEF2.2.

A systematic comparison of these two schemes has been done for a wide range of media. In many applications the results are in very good agreements (within the statistical uncertainties) and for some media (highly enriched uranium solutions with high uranium concentrations and plutonium solutions with high plutonium concentrations) a tendency of the multigroup scheme to under-estimate the k_{eff} (of about 500 pcm) was observed. This study allows to understand the origin of this discrepancy (see the following section).

The JEFF3.0 evaluation is available at this time for validation only in the multigroup scheme. The differences of the two sets of JEF2.2 ^{235}U data available (processed with two versions of NJOY) are mainly in the multigroup fission spectrum (the one processed by NJOY-94.66 having a relatively softer spectrum compared to the one processed by NJOY-89.62) and in the number of tabulated effective reaction rates (as a function of the background cross section) used in the self-shielding calculation.

V. RESULTS AND DISCUSSIONS

a. Comparison of JEF2.2 and JEFF3.0 ^{235}U evaluations

Tables 4 to 8 give the differences on the calculated k_{eff} (Δk) obtained using the two different ^{235}U evaluations (JEFF3.0 and JEF2.2). The two ^{235}U application libraries were processed using NJOY-94.66. All the other nuclides are originated from JEF2.2 and processed with NJOY-89.62. The multigroup route of CRISTAL (APOLLO2-MORET4) was used for all calculations. The standard deviation (1σ) of the difference is given between brackets (right hand side column in the tables).

These results show that the effect of ^{235}U evaluation on the calculated k_{eff} is negligible for low enriched uranium solutions and for mixed uranium and plutonium solutions. However, JEFF3.0 results are systematically lower than those of JEF2.2 for high enriched uranium solutions (the difference reach about -900 pcm), for wet uranium powders (the difference vary from -460 pcm to -840 pcm) and for uranium pins arrays (a difference of about -1000 pcm was obtained for the smallest pitch). For these media a visible trend is observed with spectrum hardness (see figure 4).

Experiments	fuel	Enrichment (%)	C_U (g/l)	$\Delta k \pm \sigma$ (pcm)
leu_sol_therm_001_01	UO_2F_2	5	978.3	-170 (141)
leu_sol_therm_002_01	UO_2F_2	4.9	452.2	130 (58)
leu_sol_therm_002_02	UO_2F_2	4.9	491.7	-10 (58)
leu_sol_therm_002_03	UO_2F_2	4.9	491.7	-90 (58)
leu_sol_therm_003_01	$\text{UO}_2(\text{NO}_3)_2$	10.2	296	50 (58)
leu_sol_therm_003_02	$\text{UO}_2(\text{NO}_3)_2$	10.2	264	-20 (141)
leu_sol_therm_003_05	$\text{UO}_2(\text{NO}_3)_2$	10.2	203	400 (141)
leu_sol_therm_003_06	$\text{UO}_2(\text{NO}_3)_2$	10.2	197	340 (141)
leu_sol_therm_003_09	$\text{UO}_2(\text{NO}_3)_2$	10.2	168	-60 (141)

Table 4 : Effect on the k_{eff} of the ^{235}U evaluations for low enriched uranium solutions
 $\Delta k = k_{\text{eff}}(\text{JEFF3.0}) - k_{\text{eff}}(\text{JEF2.2})$

Experiments	C_U (g/l)	C_{Pu} (g/l)	$\Delta k \pm \sigma$ (pcm)
Mix_sol_therm_002_058	11.05	11.88	320 (141)
Mix_sol_therm_002_059	10.78	11.73	-109 (141)
Mix_sol_therm_002_061	41.04	12.19	-149 (141)
Mix_sol_therm_003_C01	228.5	101.3	-21 (141)
Mix_sol_therm_003_C05	71.3	31.58	-249 (141)
Mix_sol_therm_003_C10	39.6	17.5	-3 (141)
Mix_sol_therm_004_065	63.38	41.69	-8 (141)
Mix_sol_therm_004_066	63.65	41.89	-29 (141)
Mix_sol_therm_004_077	262.79	172.56	-33 (141)
Mix_sol_therm_004_078	262.55	172.82	-25 (141)

Table 5 : effect on the k_{eff} of the ^{235}U evaluations for mixed homogeneous uranium and plutonium solutions. $\Delta k = k_{\text{eff}}(\text{JEFF3.0}) - k_{\text{eff}}(\text{JEF2.2})$

Experiments	C _U (g/l)	Soluble poison	C (g/l)	$\Delta k \pm \sigma$ (pcm)
heu_sol_therm_009_C01	696.42	—	—	-903 (141)
heu_sol_therm_009_C02	543.05	—	—	-919 (141)
heu_sol_therm_009_C03	348.84	—	—	-706 (141)
heu_sol_therm_009_C04	213.19	—	—	-501 (141)
heu_sol_therm_010_C01	102.06	—	—	-53 (141)
heu_sol_therm_011_C01	53.02	—	—	126 (141)
heu_sol_therm_011_C02	52.11	—	—	-160 (141)
heu_sol_therm_012_C01	21.96	—	—	-101 (141)
heu_sol_therm_013_C01	20.12	B	0	86 (141)
heu_sol_therm_013_C02	23.53	B	0.0935	-68 (141)
heu_sol_therm_013_C03	26.77	B	0.187	-350 (141)
heu_sol_therm_013_C04	28.45	B	0.23	93 (141)
heu_sol_therm_019_C01	447.3	Gd	0	-591 (141)
heu_sol_therm_019_C02	393.6	Gd	0.647	-799 (141)
heu_sol_therm_019_C03	400	Gd	1.16	-733 (141)
heu_sol_therm_018_C03	300	Gd	0	-866 (141)
heu_sol_therm_018_C09	283.3	Gd	0.977	-427 (141)
heu_sol_therm_018_C11	285.3	Gd	1.4	-720 (141)
heu_sol_therm_018_C12	279.6	Gd	1.943	-619 (141)
heu_sol_therm_001_C05	54.89	—	—	-314 (141)
heu_sol_therm_001_C07	137.4	—	—	-268 (141)
heu_sol_therm_001_C09	357.71	—	—	-726 (141)

Table 6 : effect on the k_{eff} of the ^{235}U evaluations for high enriched uranium solutions.
 $\Delta k = k_{eff}(\text{JEFF3.0}) - k_{eff}(\text{JEF2.2})$

Experiments	H/U	$\Delta k \pm \sigma$ (pcm)
leu_comp_inter_m1255	2 et 3	-842 (141)
leu_comp_inter_m1343	3	-457 (141)
leu_comp_inter_m1345	2.5	-819 (141)
leu_comp_inter_m1366	2	-526 (141)
leu_comp_inter_m2243	3	-481 (141)
leu_comp_inter_m2244	3	-513 (141)
leu_comp_inter_m2266	2	-806 (141)
leu_comp_inter_m3344	2 et 3	-654 (141)

Table 7 : effect on the k_{eff} of the ^{235}U evaluations for low enriched uranium powders (MARACAS experiments). $\Delta k = k_{eff}(\text{JEFF3.0}) - k_{eff}(\text{JEF2.2})$

Experiments	^{235}U (%)	lattices	Pitch (cm)	Soluble or solid poison	$\Delta k \pm \sigma$ (pcm)
leu_comp_therm_007_C01	4.743	Square 22 x 22	1.26	–	-1005 (141)
leu_comp_therm_007_C04	4.743	triangular 14x14x14	1.35	–	-890 (141)
leu_comp_therm_007_C06	4.743	triangular 9x9x9	2.26	–	-958 (141)
leu_comp_therm_006_C01	2.6	Square 19 x 19	1.849	–	67 (141)
leu_comp_therm_006_C09	2.6	Square 16 x 16	2.15	–	-262 (141)
leu_comp_therm_006_C18	2.6	square 19 x 19	2.293	–	-180 (141)
leu_comp_therm_035_B1	2.6	Square 21 x 21	1.956	B (70 ppm)	237 (141)
leu_comp_therm_035_B2	2.6	Square 21 x 21	1.956	B (147.7 ppm)	135 (141)
leu_comp_therm_035_C1	2.6	Square 21 x 19	1.956	Gd (64.5 ppm)	-411 (141)

Table 8: effect on the k_{eff} of the ^{235}U evaluations for arrays of low enriched UO_2 pins.

$$\Delta k = k_{\text{eff}}(\text{JEFF3.0}) - k_{\text{eff}}(\text{JEF2.2})$$

b. Experimental qualification

After establishing the effect of the new evaluation on the calculated k_{eff} we will now consider the experimental validation i.e we will compare the prediction capabilities of the two ^{235}U evaluations. As far as calculation-experiment comparison is concerned the following precautions have to be taken:

- First, high quality experiments are to be studied.
- Second, “reference” calculations are to be carried out in order to reduce calculation approximation to the lowest level possible.

In order to fulfil the first requirement we have discarded experiments for which the experimental data are still doubtful. This concerns the high-enriched uranium systems with gadolinium HEU_SOL_THERM_018 program. In fact, the calculation experiment discrepancies are unacceptably high (more than 2 %) for many combinations of codes and cross sections data (including JEF2.2 and JEFF3.0) whereas the experiment without Gd give acceptable results as well as similar programs with Gd. This is not very important since our concern is primarily ^{235}U evaluation.

To fulfil the second requirement we based our analysis on the pointwise Monte-Carlo code TRIPOLI-4. Unfortunately, at the time of this study there were no JEFF3.0 based library for ^{235}U in this code. We will thus use an approximation that assumes that the effect of the ^{235}U evaluation is code independent. As the difference $k_{\text{eff}}(\text{JEFF3.0}) - k_{\text{eff}}(\text{JEF2.2})$ was calculated with the multigroup route we will suppose that this difference is the same for TRIPOLI-4. This could be considered as valid since the effect of approximations in the multigroup route is cancelled when taking the difference and

also because qualification studies of the CRISTAL system showed that the results obtained with two routes are comparable.

To summarise, we have performed the following calculations:

- TRIPOLI-4 using JEF2.2; the corresponding results are k_{eff} (T4;JEF2.2)
- APOLLO2-MORET4 using JEF2.2; the corresponding results are k_{eff} (A2-M4;JEF2.2)
- APOLLO2-MORET4 using JEFF3.0; the corresponding results are k_{eff} (A2-M4;JEFF3.0)

And we assume that k_{eff} (T4;JEFF3.0) = k_{eff} (T4;JEF2.2) + [k_{eff} (JEFF3.0) – k_{eff} (JEF2.2)]. The last quantity between brackets being assumed to [k_{eff} (A2-M4;JEF3.0) - k_{eff} (A2-M4;JEF2.2)].

Tables 9 and 10 give the comparison between calculation and experiments for JEF2.2 and JEFF3.0. The average discrepancies for the different classes of media are given in the following table:

Class	Average (C-E) for JEFF3.0	Average (C-E) for JEF2.2
Leu_sol_therm	31 ± 200	-110 ± 170
Mix_sol_therm	161 ± 283	140 ± 76
Heu_sol_therm	-133 ± 333	249 ± 376
Leu_comp_inter	74 ± 146	711 ± 141
Leu_comp_therm	-172 ± 85	-47 ± 156
All	-45 ± 284	267 ± 384

From these tables, we can see that JEFF3.0 improves the overall average prediction and reduces the discrepancies for systems with important component of the spectrum at intermediate energies (wet powder media, tight lattices and high enriched solutions with high concentrations). In figure 5 the calculation-experiment discrepancy was normalised to the combined calculation-experiment uncertainty, i.e. the discrepancies are given in terms of total uncertainties. We have the following frequency of |C-E| as a function of intervals of ΔE (experimental uncertainty). Since the number of experiments investigated is not very large, the confidence intervals are not those of a normal distribution. In particular, the 3% frequency in the first two intervals corresponds to only one experiment among 37. Nevertheless, the results in the following table clearly indicate that JEFF3.0 is performing better than JEF2.2 since 81% of calculation-experiment discrepancies are within one experimental uncertainty compared to 51% for JEF2.2.

Interval of (C-E)	Frequency of JEFF3.0 results	Frequency of JEF2.2 results
C-E > 3 ΔE	3 %	0 %
2 ΔE < C-E < 3 ΔE	5 %	3 %
1 ΔE < C-E < 2 ΔE	11 %	46 %
C-E < 1 ΔE	81 %	51 %

Experiments	C_U (g/l)	(C-E) (pcm) JEF2.2	(C-E) (pcm) JEFF3
leu_sol_therm_003_C01	296	154	204
leu_sol_therm_003_C02	264	-66	-86
leu_sol_therm_003_C05	203	-353	47
leu_sol_therm_003_C06	197	-74	266
leu_sol_therm_003_C09	168	-215	-275
mix_sol_therm_002_058	11.05	236	556
mix_sol_therm_002_059	10.78	136	27
mix_sol_therm_002_061	41.04	50	-99
heu_sol_therm_009_C01	696.42	770	-133
heu_sol_therm_009_C02	543.05	780	-139
heu_sol_therm_009_C03	348.84	420	-286
heu_sol_therm_009_C04	213.19	-90	-591
heu_sol_therm_010_C01	102.06	190	137
heu_sol_therm_011_C01	53.02	500	626
heu_sol_therm_011_C02	52.11	280	120
heu_sol_therm_012_C01	21.96	200	99
heu_sol_therm_013_C01	20.12	-44	42
heu_sol_therm_013_C02	23.53	-310	-378
heu_sol_therm_013_C03	26.77	-546	-896
heu_sol_therm_013_C04	28.45	-281	-188
heu_sol_therm_019_C01	447.3	406	-185
heu_sol_therm_019_C02	393.6	730	-69
heu_sol_therm_019_C03	400	446	-287
heu_sol_therm_001_C05	54.89	339	25
heu_sol_therm_001_C07	137.4	402	134
heu_sol_therm_001_C09	357.71	293	-433

Table 9 : calculation-experiment discrepancy for JEF2.2 and JEFF3 evaluation.

Experiments	(C-E) (pcm) JEF2.2	(C-E) (pcm) JEFF3
leu_comp_inter_m1255	880	38
leu_comp_inter_m1343	760	303
leu_comp_inter_m1345	950	131
leu_comp_inter_m1366	480	-46
leu_comp_inter_m2243	720	239
leu_comp_inter_m2244	630	117
leu_comp_inter_m2266	630	-176
leu_comp_inter_m3344	640	-14
leu_comp_therm_006_C01	-256	-189
leu_comp_therm_006_C09	-6	-267
leu_comp_therm_006_C18	120	-60

Table 10 : calculation-experiment discrepancy for JEF2.2 and JEF3 evaluation.

Finally, we investigated the effect on the calculated k -effective of ^{235}U data processing using two versions of NJOY (94.66 and 89.62). The comparison of multigroup cross-sections did not show any significant differences except for fission spectrum as shown in figure 7. The earlier version produces a harder spectrum due to problems in the GROUPN module.

Table 11 reports the differences obtained between the two versions of NJOY for the JEF2.2 based ^{235}U libraries. We can notice that the effect of the processing is non-significant on the k_{eff} in the case of low enriched systems and mixed uranium and plutonium solutions. However, this effect can not be neglected for highly enriched uranium solutions with high concentrations. In fact, the differences can reach about 600 pcm.

These differences are approximately the same as those observed between APOLLO2-MORET4 and pointwise codes (TRIPOLI4 and MONK-7) for highly enriched uranium solutions and for plutonium solutions³. These last codes do not use the fission spectrum generated by GROUPN but sample directly from the spectrum available in the evaluation (analytical or tabulated).

Experiments	$k_{\text{eff}}(\text{NJOY-94.66}) - k_{\text{eff}}(\text{NJOY-89.62})$ (σ) (pcm)
leu_sol_therm_001_C01	340 (141)
leu_sol_therm_002_C01	160 (108)
leu_sol_therm_002_C02	20 (108)
leu_sol_therm_002_C03	380 (108)
leu_sol_therm_003_C01	40 (108)
leu_sol_therm_003_C02	-50 (141)
leu_sol_therm_003_C05	-310 (141)
leu_sol_therm_003_C06	-170 (141)
leu_sol_therm_003_C09	200 (141)
mix_sol_therm_002_058	37 (141)
mix_sol_therm_002_059	66 (141)
mix_sol_therm_002_061	278 (141)
mix_sol_therm_003_C01	74 (141)
mix_sol_therm_003_C05	-26 (141)
mix_sol_therm_003_C10	31 (141)
mix_sol_therm_004_065	75 (141)
mix_sol_therm_004_066	175 (141)
mix_sol_therm_004_077	-31 (141)
mix_sol_therm_004_078	183 (141)
heu_sol_therm_009_C01	423 (141)
heu_sol_therm_009_C02	651 (141)
heu_sol_therm_009_C03	527 (141)
heu_sol_therm_009_C04	295 (141)
heu_sol_therm_010_C01	206 (141)
heu_sol_therm_011_C01	7 (141)
heu_sol_therm_011_C02	218 (141)

heu_sol_therm_012_C01	285 (141)
heu_sol_therm_013_C01	165 (141)
heu_sol_therm_013_C02	241 (141)
heu_sol_therm_013_C03	468 (141)
heu_sol_therm_013_C04	-179 (141)
heu_sol_therm_019_C01	390 (141)
heu_sol_therm_019_C02	336 (141)
heu_sol_therm_019_C03	330 (141)
heu_sol_therm_018_C03	518 (141)
heu_sol_therm_018_C09	200 (141)
heu_sol_therm_018_C11	253 (141)
heu_sol_therm_018_C12	241 (141)
heu_sol_therm_001_C05	584 (141)
heu_sol_therm_001_C07	441 (141)
heu_sol_therm_001_C09	523 (141)
leu_comp_inter_m1255	10 (141)
leu_comp_inter_m1343	-19 (141)
leu_comp_inter_m1345	-70 (141)
leu_comp_inter_m1366	-208 (141)
leu_comp_inter_m2243	11 (141)
leu_comp_inter_m2244	175 (141)
leu_comp_inter_m2266	-180 (141)
leu_comp_inter_m3344	-306 (141)
leu_comp_therm_006_C01	-33 (141)
leu_comp_therm_006_C09	143 (141)
leu_comp_therm_006_C18	55 (141)
leu_comp_therm_035_B1	-127 (141)
leu_comp_therm_035_B2	-371 (141)
leu_comp_therm_035_C1	201 (141)

Table 11: effect on the k_{eff} of processing (NJOY-89.62 and NJOY-94.66).

VI. CONCLUSIONS

It was the aim of this paper to contribute to the validation of the new ^{235}U evaluation. Several experimental configurations were studied including low-enriched uranium solutions, high-enriched uranium solutions, mixed uranium and plutonium solutions, wet uranium powders and arrays of UO_2 pins. The following effects were investigated:

- Effect on the calculated k-effective of new ^{235}U evaluation.
- Effect on the calculation-experiment discrepancies of the new ^{235}U evaluation.
- Effect on the calculated k-effective of the NJOY processing version (89.62 or 94.66).

The main conclusions are:

- The effect of the new evaluation on the calculated k-effective is negligible for low-enriched uranium solutions and mixed uranium and plutonium solutions.

- Significant effects (up to -1000 pcm) are observed for high-enriched uranium solutions, wet uranium powders and arrays of UO₂ pins with a visible trend with spectrum hardness.
- The new ²³⁵U evaluation predicts better the experimental results than the evaluation in JEF2.2. The systematic over-predictions observed in the past for high concentrated high enriched solutions and for wet uranium powders are discarded.

The NJOY-89.62 version calculated a fission spectrum which harder than the actual one. This explains the discrepancies observed in the past between APOLLO2-MORET4 and pointwise codes.

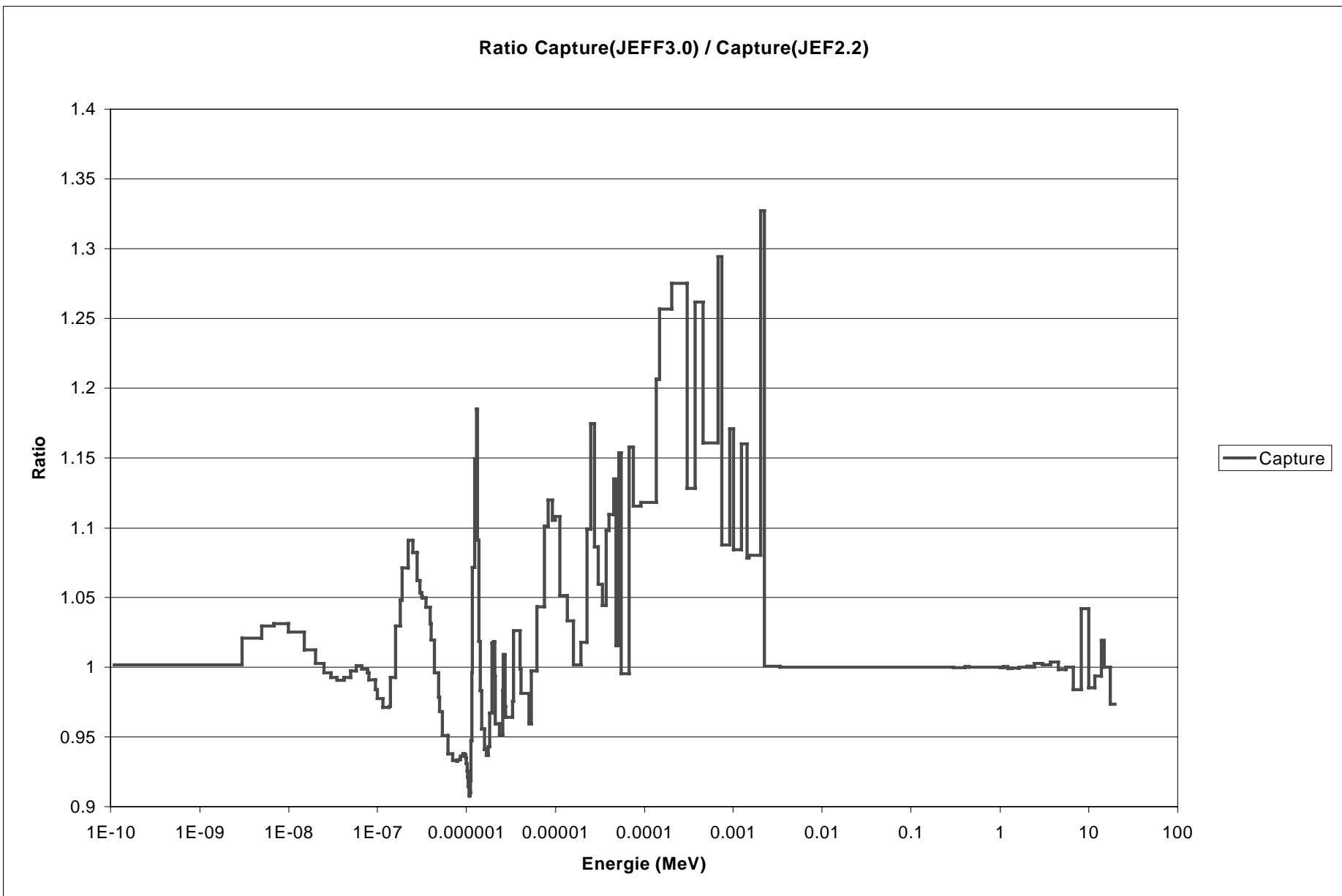


Figure 1: Ratio Capture(JEFF3.0) / Capture(JEF2.2).

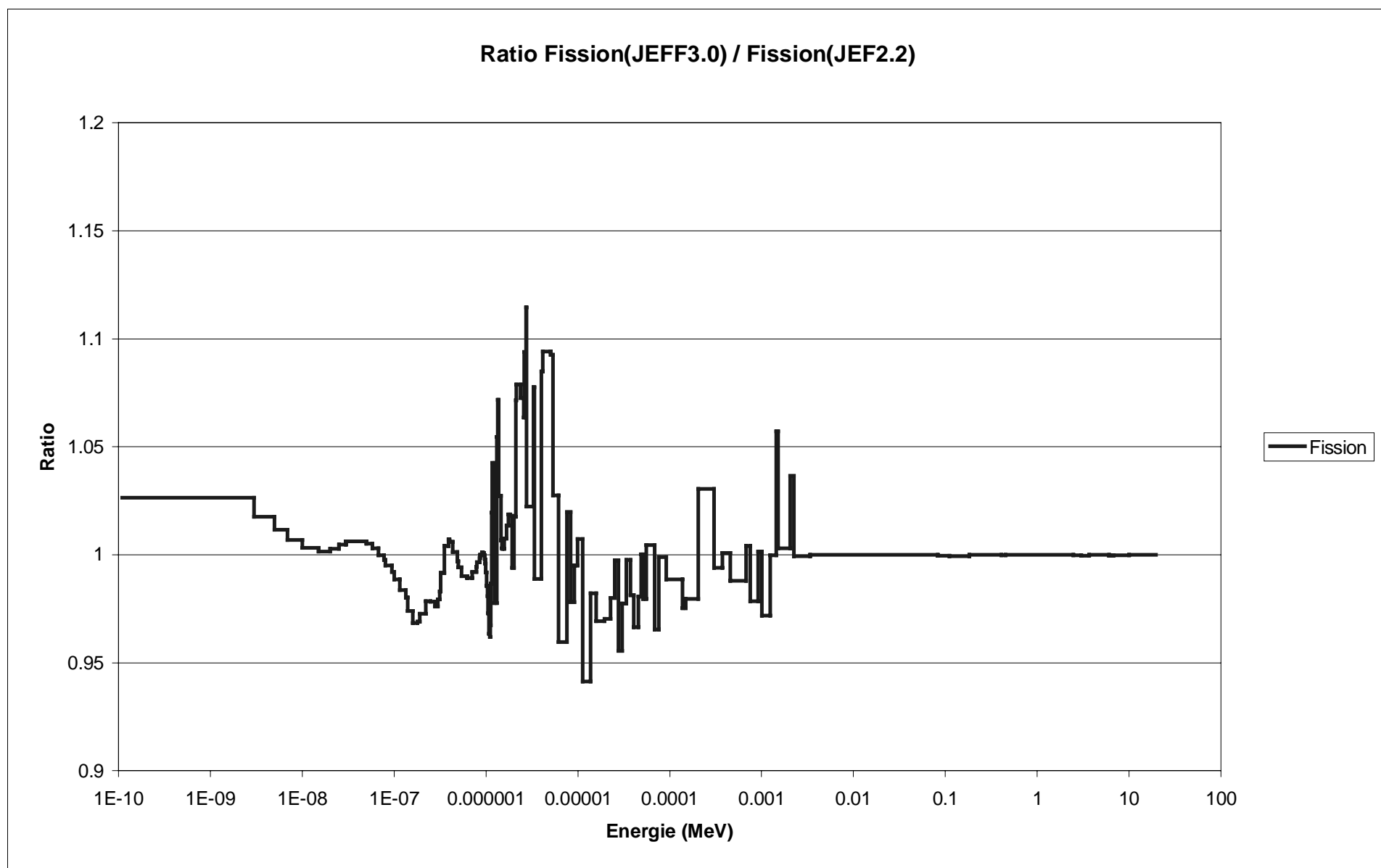


Figure 2: Ratio Fission(JEFF3.0) / Fission(JEF2.2)

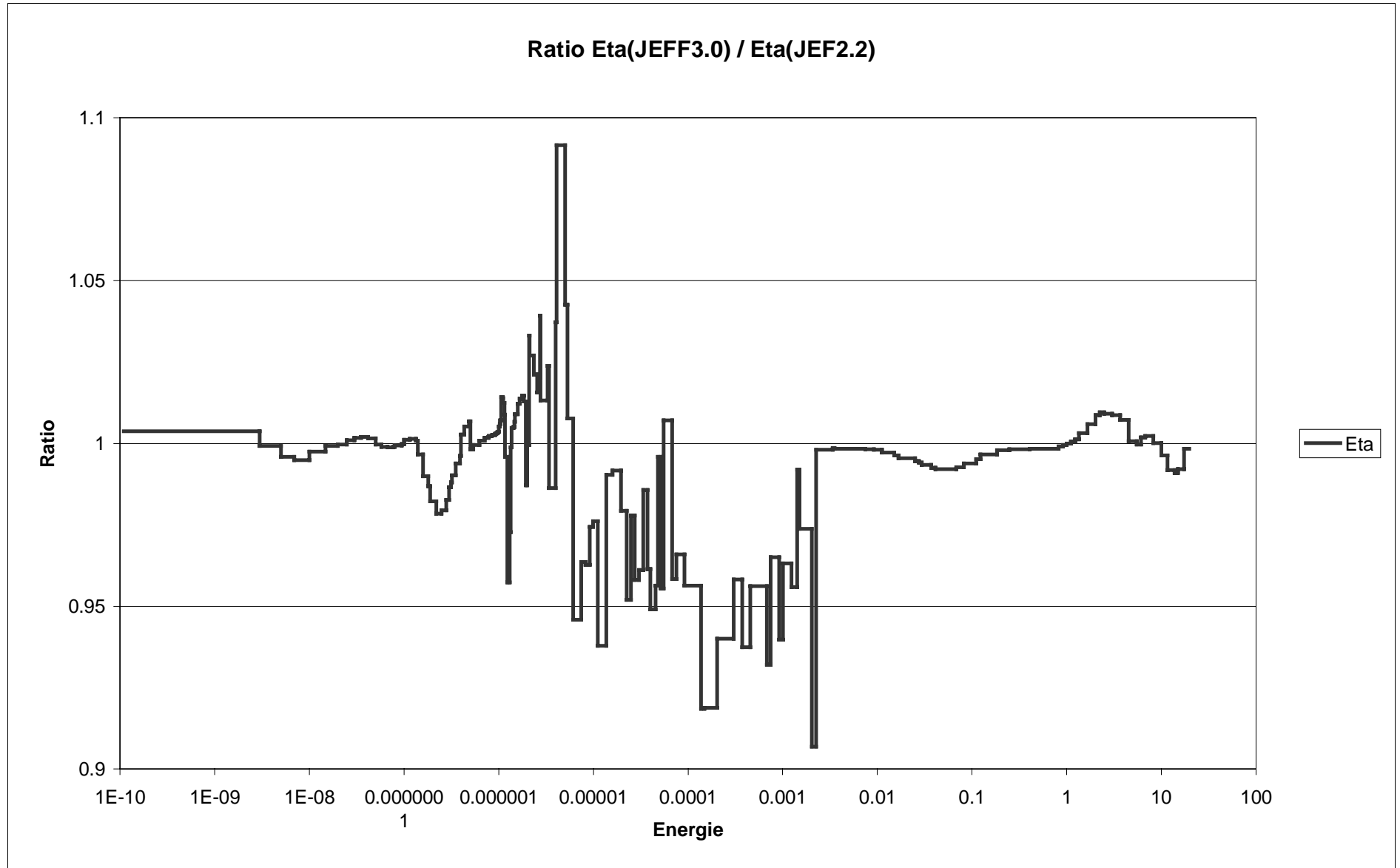


Figure 3: Ratio Eta(JEFF3.0) / Eta(JEF2.2)

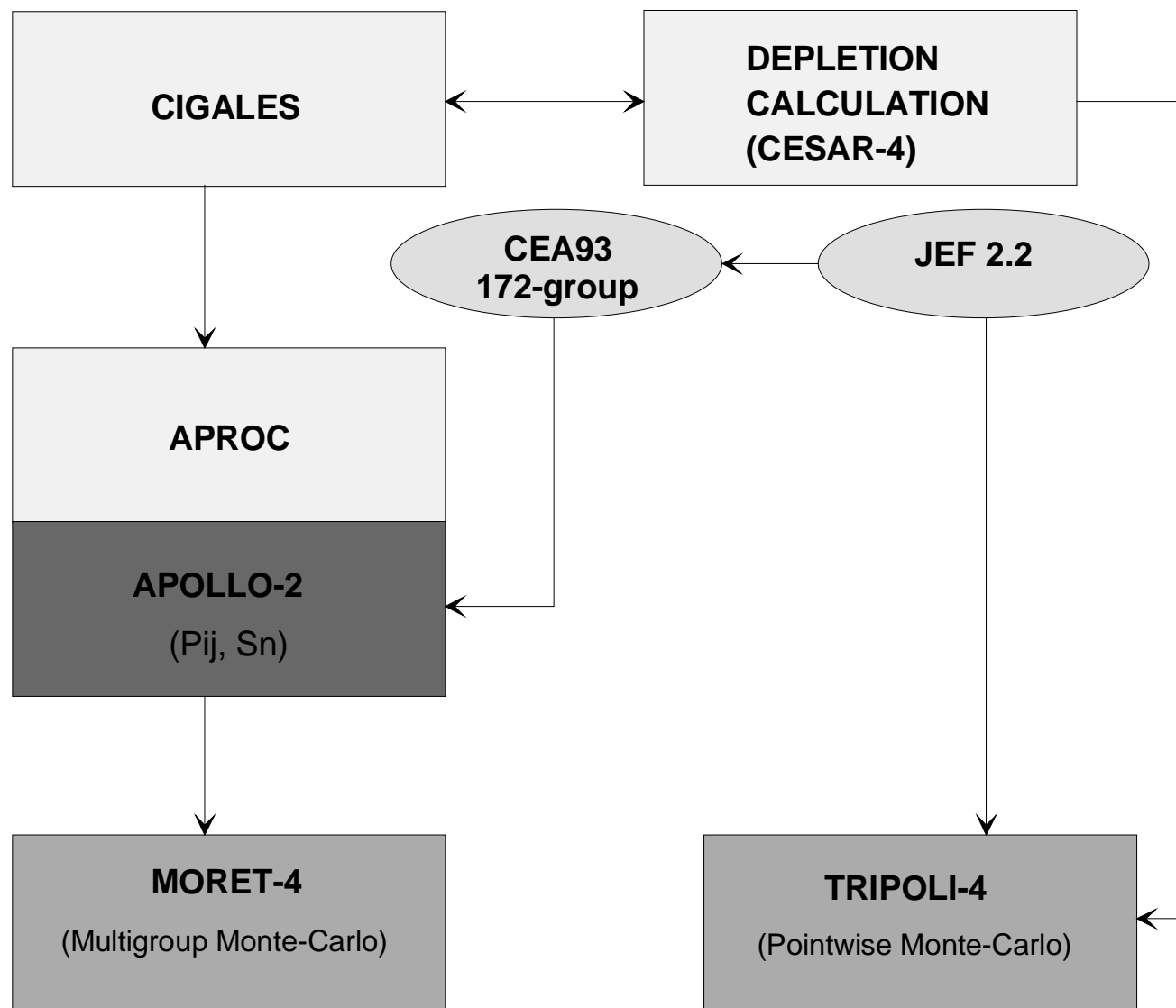


Figure 4: Flow chart of the new Criticality Package CRISTAL

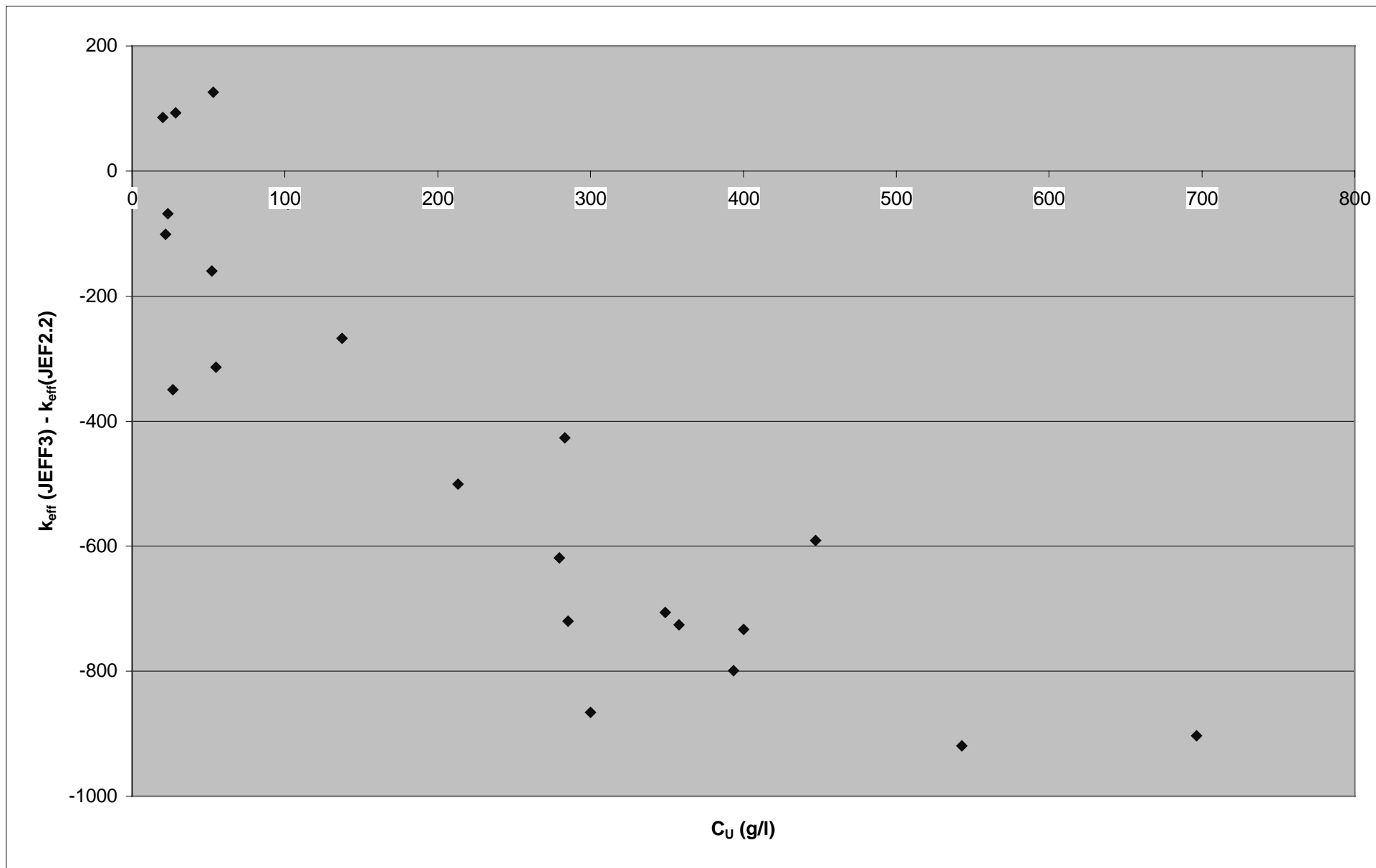


Figure 5 : effect on the k_{eff} of the ^{235}U evaluations: JEF2.2 JEFF3 for high enriched solutions.

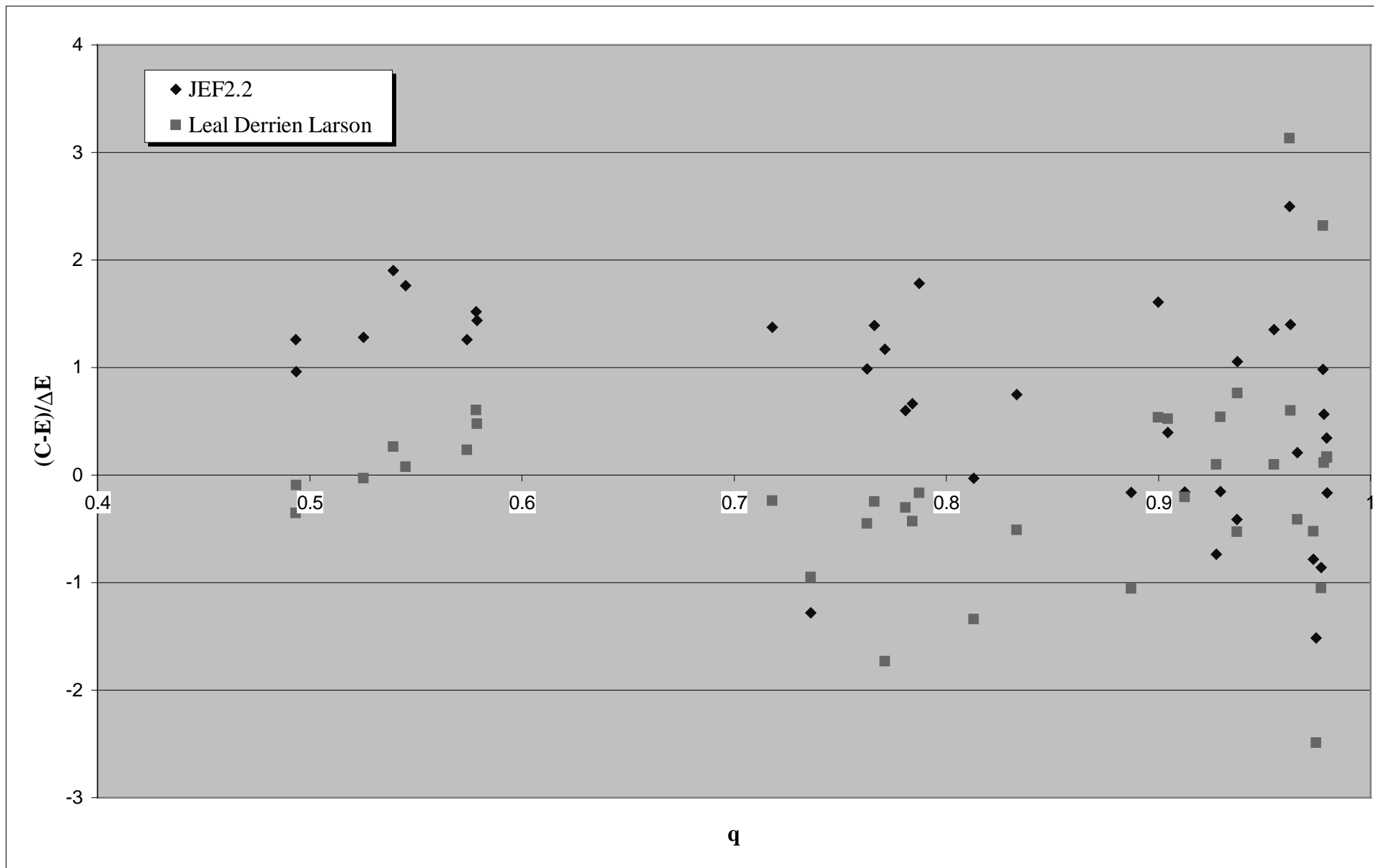


Figure 6 : discrepancies between experiments and calculations for the ^{235}U evaluations (JEF2.2 and JEFF)

Comparison of ^{235}U fission spectrum processed with two NJOY versions

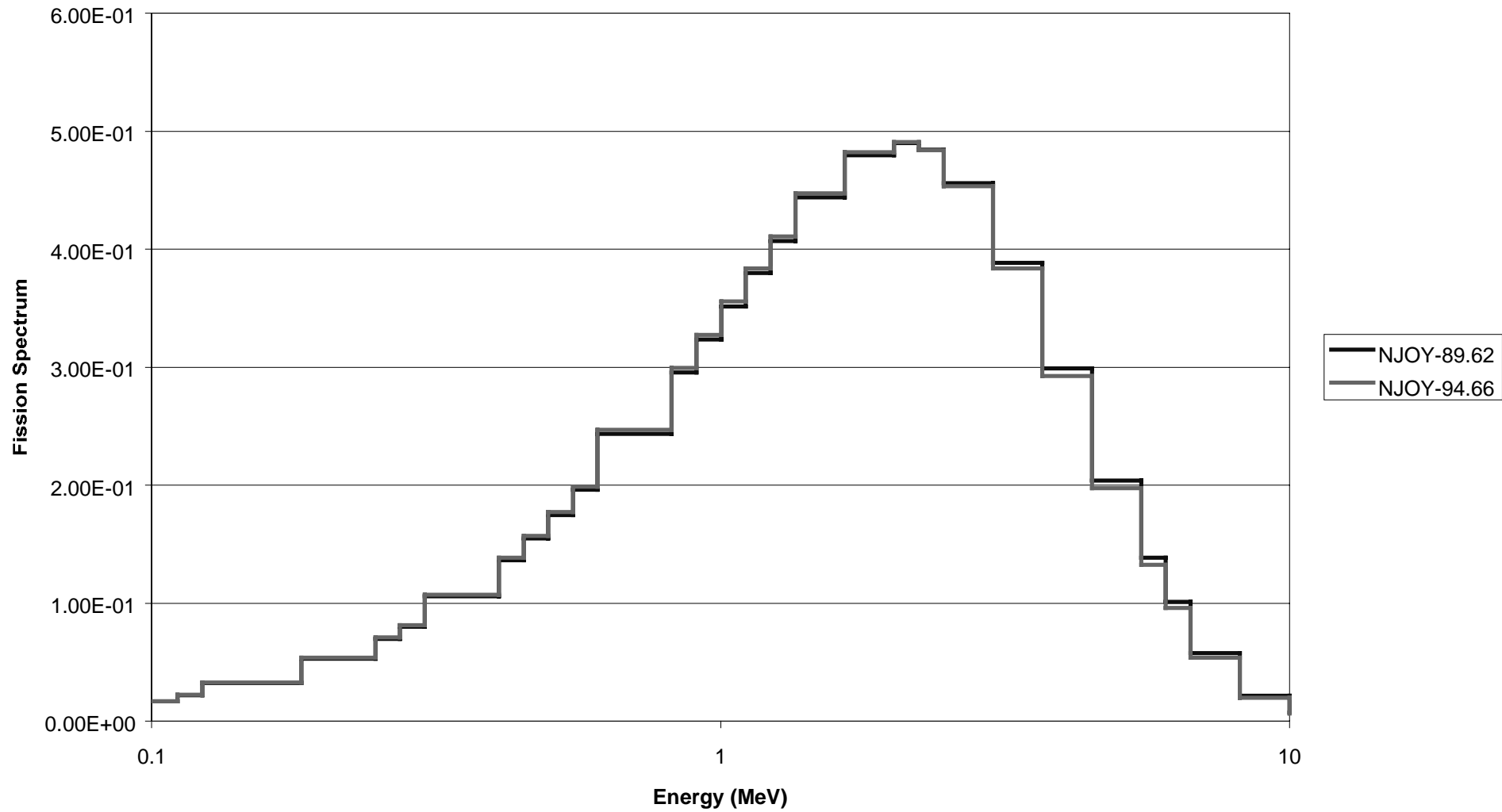


Figure 7 : discrepancies between experiments and calculations for the ^{235}U evaluations (JEF2.2 and JEFF)

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