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INTEGRAL DATA TESTING FOR THERMAL REACTORS AND FEEDBACK INTO JEF2

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INTRODUCTION

Nowadays, the calculation of a nuclear reactor core is generally performed by solving the Boltzmann equation. According to the computer code we solve the integral form or the integro-differential form of the transport equation. But in any case we need numerous numerical data : the geometrical and chemical data, and the neutron and nuclear data. The former data represent the dimensions of the cell and the core, the chemical and isotopic composition of the fuel, the structures and the moderator. They are generally known with a good accuracy. The latter data represent the neutron cross sections and the nuclear properties of the various nuclides. They are not always known with an accuracy as good as the reactor physicist wishes. The neutron data are generally deduced from direct nuclear measurements. These measurements give the variation of the nuclear properties of the nuclides versus the incoming neutron energy : they are the differential experiments. Generally, the shape of the cross sections can be more or less well achieved. But very often, it is difficult to measure the absolute magnitude of the nuclear data with the accuracy required by the physicist needs. Some of the best estimated values of the evaluated files can have an uncertainty which is too large. To improve the knowledge of the nuclear parameters we must use another type of experiment : the integral experiments. In this kind of experiments we use a mock-up of a reactor or the reactor itself and we measure some synthetic parameters which are representative of the neutron properties of the cell or of the reactor for the actual neutron spectrum. For example, we can measure criticality factor, buckling, reaction rates or irradiated fuel composition.

If we choose integral experiments with very simple geometries and asymptotic spectrum such as uniform lattices or homogeneous media we can perform the calculation of these experiments without numerical approximations. In these conditions, it is possible to use very sophisticated options of the reactor computation codes.

So the difference between the computed values of the synthetic parameters and the experimental ones can be attributed to the inaccuracy of the neutron data used in the calculation. These neutron data depend on the evaluated files but also on the processing. It is very important to handle very carefully the processing codes which generate the multigroup cross sections used by the reactor physics. The second important thing is to solve the Boltzmann equation without bias. For this it is necessary to check the geometrical description of the cell and the energy mesh of the multigroup cross sections for each integral experiment. Only if all these conditions are achieved, we can deduce modifications of the neutron data from the difference between the computed and the measured values of a set of integral experiments. For this purpose, we can use the tendency research method [1,2]. In this method, the difference between the computed and the measured values of an integral parameter, effective multiplication coefficient for example, is expressed as a linear function of the cross section modifications. The cross section modifications are obtained by a least square computation. Therefore, it is necessary to have different sensitivity coefficients. For the thermal neutron reactor this condition is achieved by using multiplying media with different kind of moderator : heavy water, light water and graphite, and for each moderator we use several fuel over moderator ratios and various fuel enrichments. In addition, the number of integral experiments must be much higher than the number of sensitive neutron data.

In the following sections, we will describe the main synthetic parameters which govern the physics of the thermal neutron reactors, the set of integral experiments which were used in this study and the results obtained in the case of the JEF2 benchmarking. The fundamentals of the tendency research method are briefly recalled in the appendix.

SENSITIVE NEUTRON DATA

To validate the neutron data, with integral experiments, we must use multiplying media with a very simple geometry. Consequently, we can perform the computation of a unique cell or of a fuel assembly in its asymptotic neutron spectrum. In these conditions we can use the more sophisticated options of the reactor physics code and this without geometrical approximation. For the thermal reactor benchmarking of JEF2, we used the recent Apollo2 code [3]. In Apollo2, which solves the integral Boltzmann equation by the collision probability method in the multigroup approximation, the resonance range is treated with an improved self-shielding formalism [4,5]. Now, it is possible to use several self-shielding areas inside the fuel pin and the equivalence procedure between the heterogeneous lattice and an homogeneous medium can be made group by group with various slowing down models. For this work, we used six different self-shielding areas in the rods and the equivalence was performed with the statistical model for the high energy resonances and the wide resonance approximation for the low energy resonances. These new possibilities have a significant impact on the benchmarking results in the resonance energy range because the effective integrals are computed with a better accuracy than in the past, where we were able to use only one self-shielding domain [6].

The total energy range is described by 172 groups. That is to say, that in the neutron library, each cross section of each isotope is represented by 172 values and that the various transfer matrices have a very high order. With integral experiments, it is not possible to obtain informations for all the cross sections and all the groups and for each matrix element. But the differences between the computed values of integral results and the measured ones can be explained with a smaller number of parameters which globally represent the neutron behaviour of a multiplying medium. They are the synthetic parameters and it is for these parameters that we will be able to deduce informations. The nature and the number of the synthetic parameters depend on the reactor types which are studied. As far as the heavy nuclei are concerned and in the case of thermal neutron reactors, we can divide the energy range in three domains :

- The energy range above 50 keV which is characterized by smooth variations of the cross section. It is mainly the fission cross sections which are important in this domain.

- The resolved and unresolved resonance energy range between 1 eV and 50 keV, in which both the resonance parameters and the self-shielding formalism are involved. The effective integrals constitute the convenient parameters in this domain.

- The thermal and subthermal energy range below 1 eV where the cross section have also a smooth behaviour. For these energies, the cross section shapes are generally well known through the differential measurements. Consequently, we have adopted the cross section shapes of the evaluated file, JEF2 in our case, and have chosen the magnitudes of the cross section for a 0.025 eV neutron as sensitive parameters.

- For the plutonium 240, the low energy range is governed by the 1.056 eV resonance and the most important parameters are the radiative capture width of the resonance and the thermal absorption cross section.

Another quantity is important for the fissile nuclei, the average number of neutrons which are emitted in a fission, nu-bar. As in the thermal neutron reactor it is mainly the low energy range which is preponderant, we have adopted the nu-bar shape of the evaluated file and chosen as synthetic parameter the nu-bar value for a 0.025 eV neutron.

For the moderator (light water, heavy water or graphite), the low energy behaviour can be characterized by the thermal absorption cross section and the slowing down and diffusion properties by the migration area. The thermal absorption of the heavy water is too few sensitive to be kept as a synthetic parameter.

Finally 29 synthetic parameters were taken into account for the validation of JEF2. They are given in table I.

INTEGRAL EXPERIMENTS

Three essential conditions must be satisfied to obtain accurate tendencies on the basic neutron data : very simple experiments with an asymptotic neutron spectrum, different sensitivity coefficients and the possibility to disconnect the effects of uranium from the ones of plutonium and thorium. The asymptotic neutron spectrum can be observed in critical facilities which used cells with only one kind of fuel. In this case, the buckling can be define without ambiguity and the reactor calculation can be made with a one cell computation. If this buckling is measured with a very good accuracy, this type of clean experiment is very interesting for the tendency research. Unfortunately they are scarce. The homogeneous experiments for which we known exactly the critical composition and the geometrical dimensions are also interesting because some of them contain only plutonium and for that they are not perturbed by uranium. At last various sensitivity coefficients can be obtained with lattices moderated by heavy water, light water or graphite and several moderating ratios.

The integral data set which we used for the JEF2 benchmarking can be split into three parts : the multiplying media which only contain uranium (uranium 235 alone or a mixture of uranium 235 and uranium 238), the ones which contain plutonium and finally the lattices representative of the thorium cycle. In each case we had at our disposal experimental value of the buckling which corresponds to the fondamuntal mode. The various multiplying media which cover a wide range of neutron spectra, from the well thermalized lattices (95% of this neutron are slowed down below 2.8 eV) to the hard spectra of the tight pitch lattices (only 25% of the neutron are slowed down below 2.8 eV) are briefly described below.

a) **Uranium**

Independantly of the moderating ratio, the uranium lattices depends on the nature of the moderator and the enrichment in uranium 235. They are :

- 7 heavy water lattices with natural uranium metallic fuel. These very thermalized media are mainly sensitive to the low energy range of the cross sections.

- 4 natural uranium and graphite lattices. They are also sensitive to the low energy range but in association with the preceding experiments they allow to separate the effect of the heavy water from the one of the graphite.

- 1 light water moderated lattice with metallic fuel containing 1,3% of uranium 235.

- 9 uranium dioxide lattices containing from 1,4 % to 2,7 % of uranium 235 and moderated by light water. In these experiments are included the well known TRX benchmarks.

- 6 uranium dioxide lattices for which the epithermal range was enhanced by using various tight pitches.

- 9 recent french critical experiments which were performed in the frame of the light water reactor studies.

- 2 homogeneous multiplying media of Oak Ridge which used 93% enriched uranium. These experiments are very interesting because they are very few sensitive to uranium 238.

- 1 critical facility with bucklings mesured between 20°C and 210°C : the swedish experiment KRITZ.

b) **Plutonium**

The plutonium fuels are characterized by two important parameters : the amount of plutonium or the plutonium over uranium ratio and the isotopic composition of the plutonium. The fuel can contain a more or less important quality of plutonium 240 and the lattices can be more or less sensitive to this isotope. Consequently we have used multiplying media with various plutonium over uranium ratios and various isotopic compositions.

The integral experiments used for this study are :

- 6 heavy water moderated lattices with metallic fuel which only contain 0,4% of plutonium with 6% of isotope 240.

- 14 light water moderated lattices which contain from 1,5 to 4,0% of plutonium. The proportion of plutonium 240 is equal to 8 or 22%.

- 5 homogeneous media with 3 and 5% of plutonium 240. These multiplying media are important for the plutonium qualification because they do not contain uranium.

- 3 tight pitch lattices with 11% of plutonium This experiments were performed in France, in the frame of the plutonium recycling studies.

c) Thorium cycle

Since several years the thorium cycle has not a high priority. The experiments which are related to this cycle are generally old, scarce and not always accurate enough. The uranium 233 and thorium validation is based on four sets of critical or exponential experiments.

- 2 light water moderated lattices the fuel of which is a mixture of uranium 235 and thorium. They are critical experiments.

- 7 exponential experiments in which the fuel is composed of uranium 233 and thorium. The moderator is light water.

- 5 exponential experiments which used the same uranium 233 and thorium fuel but heavy water as moderator.

- 2 homogeneous media composed by a solution of uranium 233 nitrate in light water.

Finally we had at our disposal 83 buckling measurements. To these integral experiments we added results coming from spent analysis and spectrum indices which gave informations about the radiative capture cross sections or the radiative capture over fission ratios of various fertile and fissile nuclei.

RESULTS AND ANALYSIS

All the eighty-three critically factor computations were used in a single least square calculation. For a first run, the twenty-nine synthetic parameters were considered as free parameters. A detailed analysis of this preliminary result showed that the observed tendencies were small and inaccurate in the case of several parameters. The statistical uncertainties deduced from the least square calculation were much greater than the magnitude of the suggested changes. Consequently, these small modifications can be considered as having no physical meaning and there is no inconvenience to fix these parameters and to keep their initial JEF2 values. Then a second least square calculation was performed with a reduced number of free parameters. In comparison with the first computation we observe a very small increase of the chi-square. This small increase justifies the reduction of the free parameter number.

As far as the thermal neutron reactors are concerned the tendency research suggests meaningful modifications for only a small number of sensitive parameters : the migration area of the light water and of the heavy water, the effective integral of the fertile nuclei uranium 238 and thorium 232 and the thermal data of uranium 233. For all the other parameters, the required modifications are very small and the best estimated values are very close to the initial values of the file. If we take into account the suggested modifications, the computation of the whole set of integral experiments is satisfactory as it can be seen on figures 1 through 3. On these figures we have displayed the difference between the computed value k_{eff} and experimental value which is equal to unity. The error bars represent the experimental uncertainty. Each integral experiment is identified by the slowing down density q. It is the number of neutrons which become thermal for one emitted fission neutron. This quantity is representative of the neutron spectra. The high values of q correspond to the soft spectra of the well thermalized lattices (mainly with heavy water or graphite as moderator) and the low values to the hard spectra of the tight pitch lattices (light water with a low moderator to fuel ratio). The figure 1 is relative to the multiplying media which contain only uranium. The average discrepancy of K_{eff}-1 is equal to -14.10^{-5} and the dispersion is equal to 482.10^{-5}. We do not observe any shift as a function of the spectrum hardness. On figure 2, we have the same representation for the multiplying media which contain, only plutonium or a mixture of plutonium and uranium. In this second case, the average k_{eff}-1 is $(182 \pm 535).10^{-5}$. For the integral experiment relevant to the uranium 233-thorium cycle the comparison is displayed on figure 3. The average k_{eff}-1 is equal to $(-275 \pm 640)10^{-5}$. For this case the dispersion is higher than for the uranium and plutonium cycles. But the integral experiments are old and not always accurate enough because they are mainly exponential experiments. For the whole set of critically factors the average deviation is $(-5 \pm 550)10^{-5}$. The statistical distribution of the reduced residual deviations $|k_{eff}-1|/\Delta K_{eff}$ is given in figure 4.

The dotted line is the Gauss distribution. We can observe a slight difference with a pure Gauss distribution. There is an excess of large deviations. This can be explained by the fact that some experimental error bars are likely too small. Nevertheless the results of the tendency research seem very satisfactory. They are the following ones.

For the major fissile nuclei uranium 235 and plutonium 239 the requested modifications are very small and within the error bars. Consequently, it is possible to keep the initial values of JEF2 for the thermal neutron reactors. The tendency research values are given in table II and we can see that the agreement with the initial values is very good. In the case of uranium 233, the situation is less satisfactory because the analysis of the integral experiments suggests important modifications of nu-bar and of the radiative capture cross section. For these two parameters the obtained values are incoherent with the initial ones.

For the fertile nuclei, uranium 238 and thorium 232, the problem is a little bit more complicated than for the fissile nuclei. The sensitive parameters are the effective integrals and the computed value of these quantities is strongly linked to the formalism and approximations which are used in the reactor core calculations. Even with the very sophisticated options of Apollo2 that we have used, the analysis of the integral experiments suggests a slight decrease of the fertile nuclei effective integral as it can be seen in table III. Let us notice that the uncertainties which are associated with these modifications remain important. They do not allow to conclude with assurance that the basic data of the fertile nuclei must be revised. Further investigations are needed before to endorse such a requirement.

For the other actinides, the sensitivity of the integral experiments are not important enough to obtain significant modifications of the neutron data.

CONCLUSION

The use of integral experiments and of the tendency research method, or a similar one, is a very efficient tool to improve the basic neutron data. It is a complementary approach to the microscopic cross section measurements and it gives important informations to the evaluators. In the case of JEF2 it was taken into account the most recent differential measurements of the major actinides and the benchmarking results of the preliminary version of the file was also used. We have now at our disposal a file which gives entire satisfaction for uranium 235 and plutonium 239 as far as thermal neutron reactors are concerned. No modification of the low energy part of these two evaluations is needed. For uranium 233 we observe a significant discrepancy between the thermal data deduced from the differential measurements and the values obtained with the integral experiments. In case of thorium cycle revival, a revision of the uranium 233 evaluation will be probably necessary, jointly with new and more accurate integral experiments.

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APPENDIX

FUNDAMENTALS OF THE TENDENCY RESEARCH METHOD

For each integral experiment (criticality factor, reaction rate ...), we know the experimental result Y_i and the measurement uncertainty E_i. In any case, we can compute the same quantity which is a function of the neutron parameters x_k. The result of this calculation is $F_i(\ldots, x_k, \ldots)$. If we change the value of the neutron parameter x_k, which becomes $x_k + \Delta x_k'$, the result of the computation is now $F_i(\ldots, x_k + \Delta x_{k'}, \ldots)$.

The principle of the tendency research method is to choose the modification Δx_k of the neutron parameters in such a way that the quantity.

$$Q = \sum_i \frac{1}{E_i^2} \left[Y_i - F_i(\ldots, x_k + \Delta x_k, \ldots)\right]^2$$

for all the set of integral experiments becomes minimum. Nowadays the magnitude of the main neutron cross sections are more or less well known. So, the modifications Δx_k are expected to be small and we can make a first order expansion of the computed value.

$$F_i(\ldots, x_k + \Delta x_k, \ldots) = F_i(\ldots, x_k, \ldots) + \sum_k \Delta x_k \frac{\partial F_i}{\partial x_k}$$

We can also replace the partial derivatives by the sensibility coefficients

$$S_{ik} = \frac{\Delta f_i}{\Delta x_k}$$

These sensibility coefficients (variation of the integral quantity F_i for a one per cent change of the parameter x_k) can be computed by the perturbation theory or a variational method.

With these assumptions we must now minimize the quantity

$$Q = \sum_i \frac{1}{E_i^2} \left[Y_i - F_i(\ldots, x_k, \ldots) - \sum_i S_{ik} \Delta x_k\right]^2$$

or if ΔY_i represents the difference between the experimental result and the computed value for the integral experiment i

$$Q = \sum_i \frac{1}{E_i^2} [\Delta Y_i - \sum_k S_{ik} \Delta x_k]^2$$

The minimization is done with the least square method. That is why, if we want to determine the modification Δx_k with a good accuracy, it is absolutely necessary to use a set of integral experiments for which the sensitivity coefficients are as different as possible. We can obtain different sensibility coefficients by using integral experiments corresponding to various types of reactors.

From the mathematical point of view, the least square calculation leads to the Δx_k values which minimize the quantity Q. But we must take two remarks into account. First, the Δx_k are assumed to be small (don't forget that we have made a first order expansion of F_i). Secondly the cross sections are measured by differential experiments with an experimental uncertainty ϵ_k. The Δx_k must be lower or of the same order than ϵ_k. This is why, instead of minimizing the Q value, we prefer minimize the following quantity :

$$Q' = \sum_i \frac{1}{E_i^2} [\Delta Y_i - \sum_k S_{ik} \Delta x_k]^2 + \lambda \sum_k \left(\frac{\Delta x_k}{\epsilon_k}\right)^2$$

In this expression λ is a free parameter which represent the importance given to the microscopic data in the tendency research.

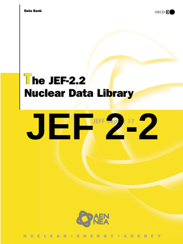


TABLE I

SENSITIVE PARAMETERS FOR THERMAL NEUTRON REACTORS

Nucleus	Thermal Range	Resonance Range	High energy range
U 233	ν, σ_f, σ_a	$I^a{}_{eff}$, $I^f{}_{eff}$	-
U 235	ν, σ_f, σ_a	$I^a{}_{eff}$, $I^f{}_{eff}$	-
U 238	-	$I^a{}_{eff}$	σ_f
Pu 239	ν, σ_f, σ_a	$I^a{}_{eff}$, $I^f{}_{eff}$	-
Pu 240	σ_a	Γ_γ	-
PU 241	ν, σ_f, σ_a	-	-
Th 232	-	$I^a{}_{eff}$	σ_f
H_2O	σ_a	M^2	-
D_2O	-	M^2	-
C	σ_a	M^2	-

TABLE II

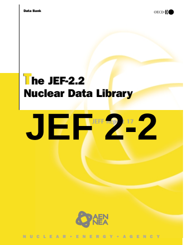
FISSILE ACTINIDE THERMAL DATA

		Initial JEF2 value	Tendency Research result
U 235	ν	2.437	2.439 ± 0.004
	σ_f	582.5	582.2 ± 1.0
	σ_c	98.8	99.1 ± 1.0
Pu 239	ν	2.877	2.872 ± 0.007
	σ_f	747.2	745.4 ± 2.0
	σ_c	270.2	273.8 ± 3.9
U 233	ν	2.498	2.480 ± 0.004
	σ_f	525.1	525.4 ± 1.1
	σ_c	45.9	50.8 ± 2.0

TABLE III

FERTILE ACTINIDE EFFECTIVE INTEGRAL MODIFICATIONS

	ΔI_{eff} (barn)
U 238	- 0.20 ± 0.11
Th 232	- 0.16 ± 0.08



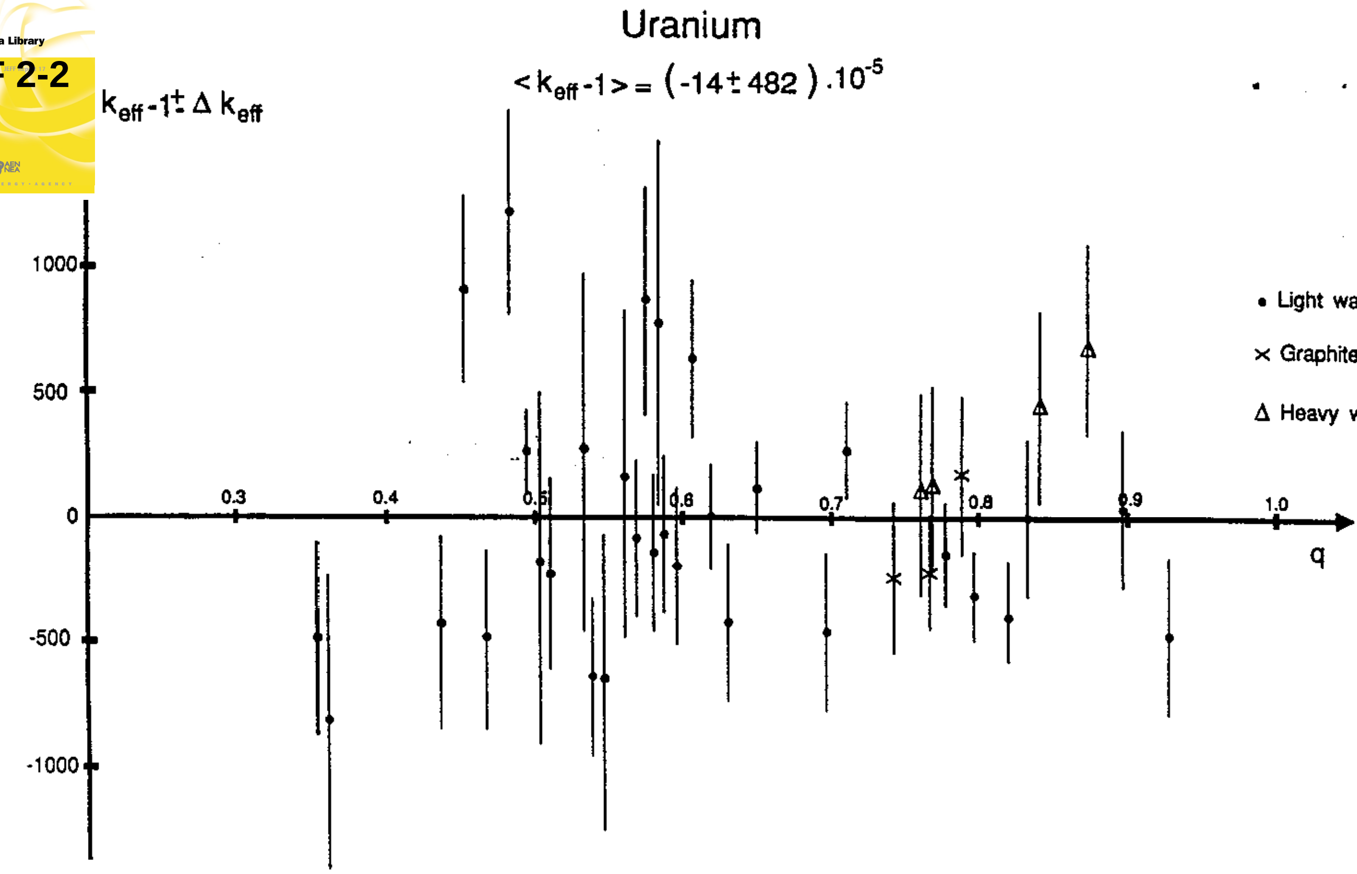


Figure 1

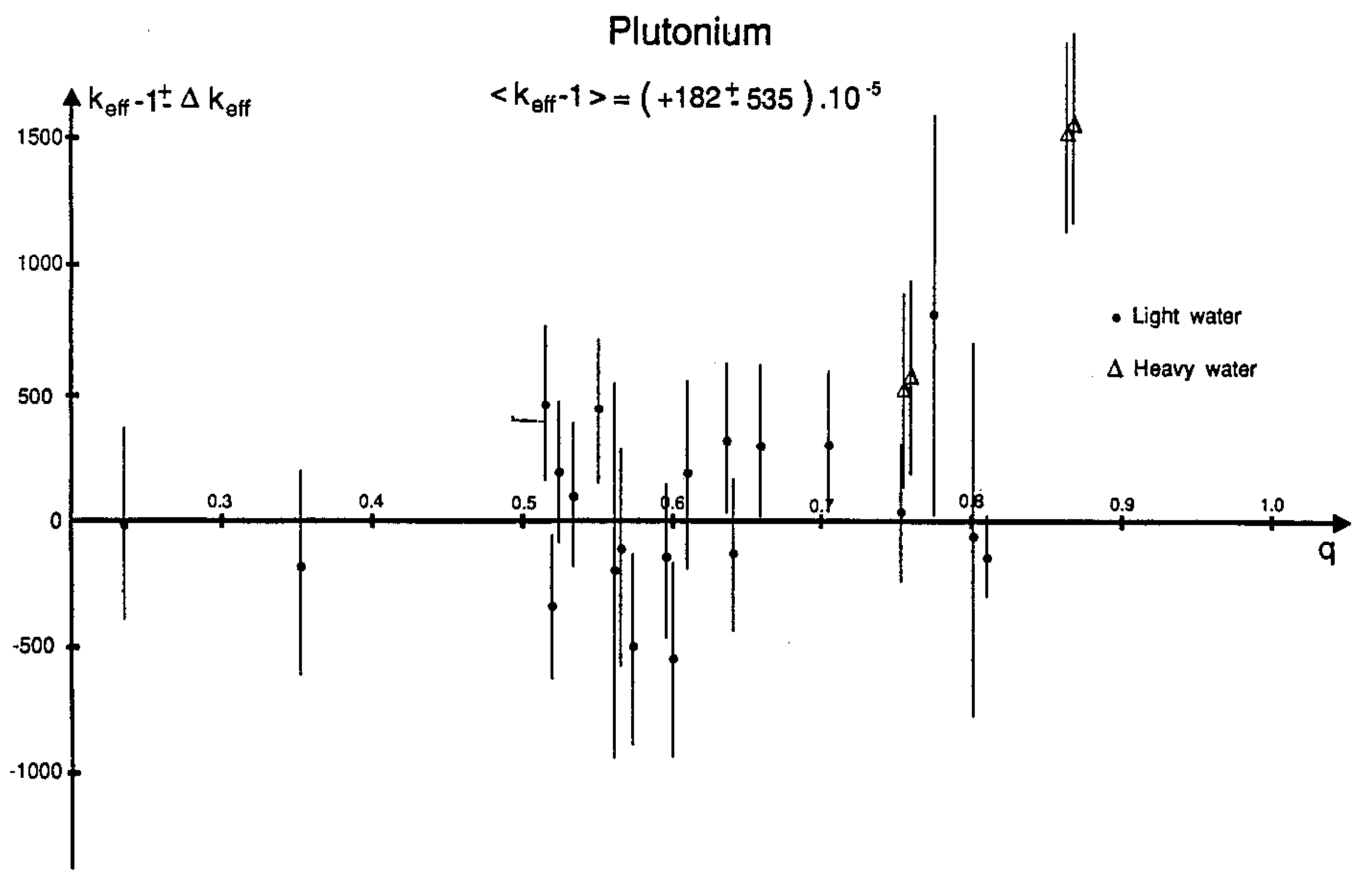


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Figure 2

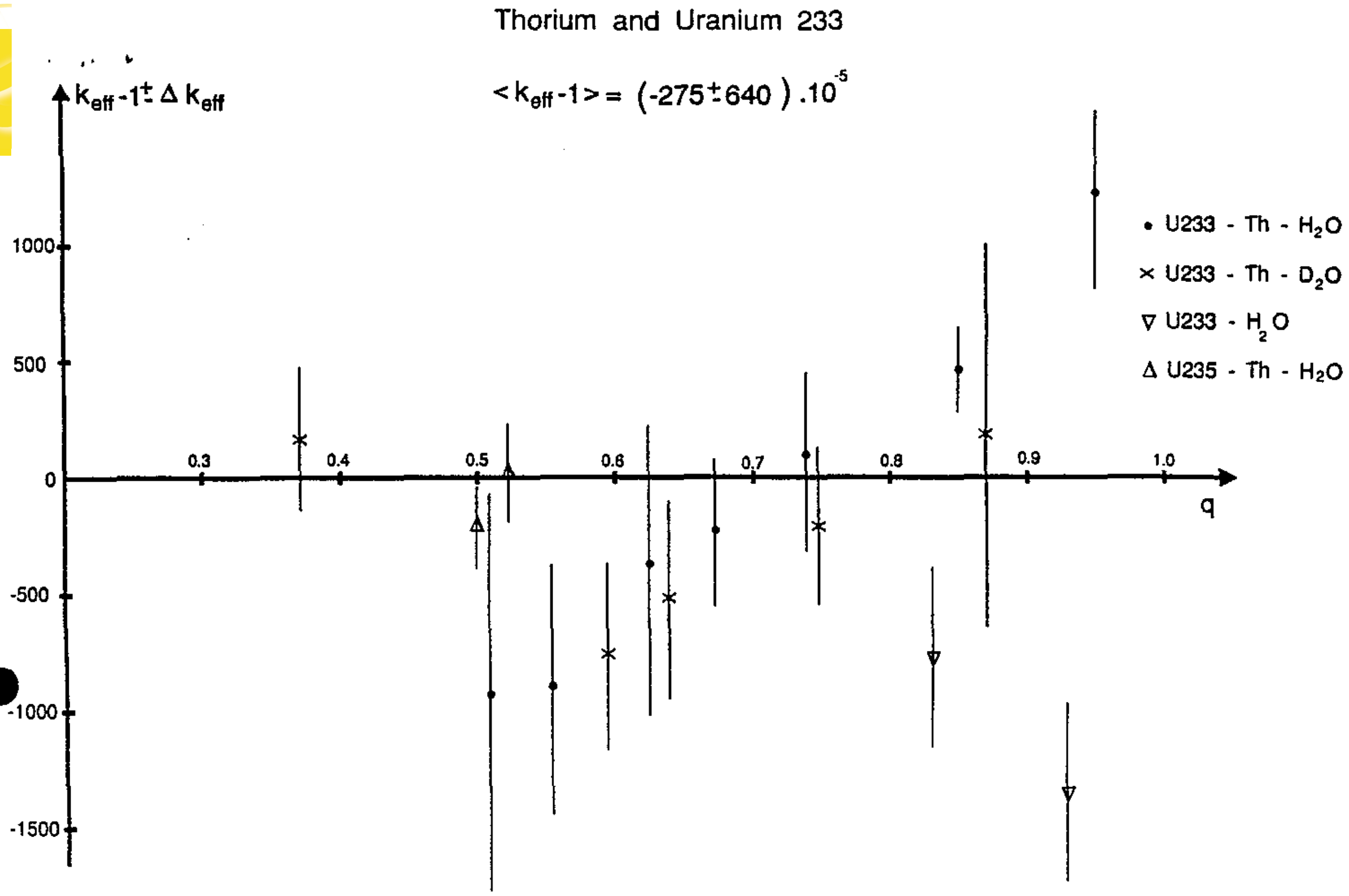

Figure 3

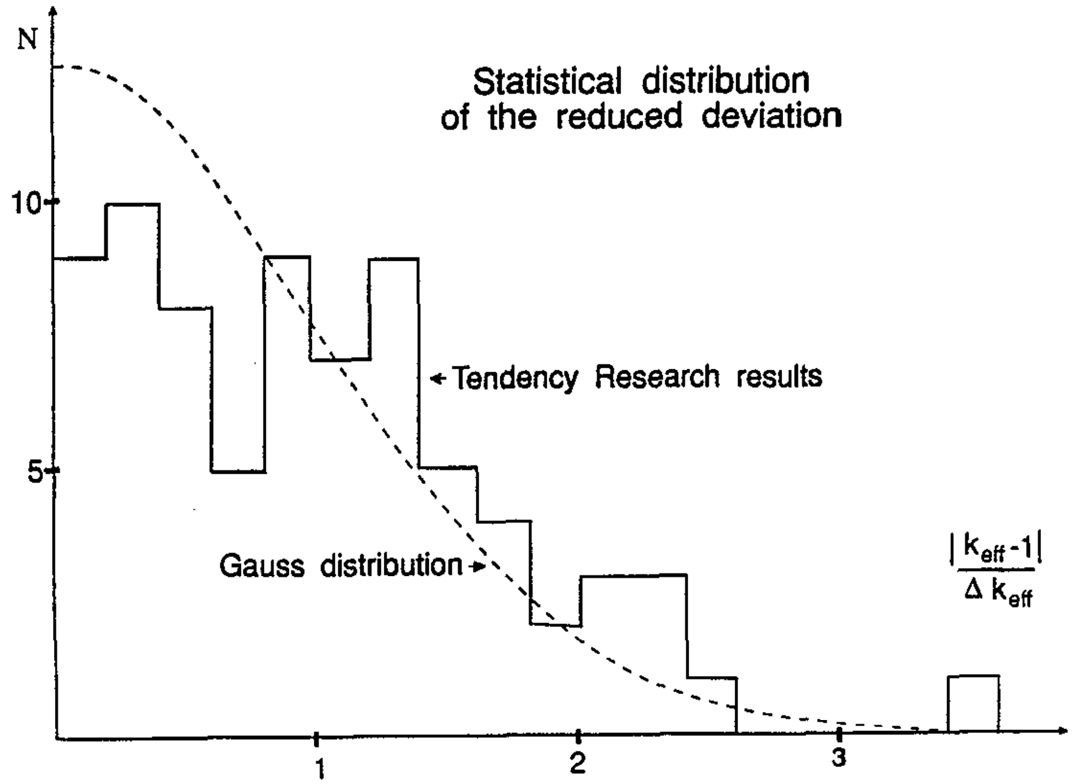

Figure 4

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