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JEF2 VALIDATION

Global analysis - Problems encountered
Provisional conclusions at the date of 14/06/1993

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GENERAL FRAMEWORK

The objectives, the philosophy and the methodology of the JEF2 benchmarking have been broadly described in another paper [1].

The benchmarking is based on a group data adjustment, which provides the modifications $d\sigma_g$ to be applied to the group constants derived from the files being validated.

This means :

- Data processing.

  This has been done basically with a validated NJOY/THEMIS version.

- a choice of energy schemes for the integral data calculations.

An European consensus has been made in favour of a 1968 g scheme for fast systems, of a 172 g scheme for thermal systems, of 175 g VITAMIN-J scheme for systems involving the transmission of bulk media by neutrons. These schemes are consistent.

- A choice of an adjustment method and of an energy scheme.

We have chosen the method of the statistical adjustment based on the minimization of a maximum likelihood estimator using the LAGRANGE multipliers. The code used is the code AMERE which is the French version of the AMARA code [2].

The energy scheme is a 15 group scheme consistent with all the others here above mentioned.

- A choice of an Integral data set to be used in the benchmarking based on a definition of what is a benchmark experiment.

In order to obtain reliable correct information on the energy dependence of $d\sigma_g$ and to separate the effects of different cross-section types it is desirable to have as many experiments with different hardness indices as possible and for a given integral experiment as many parameters as possible (K_{eff}, B^2_m, indices, response functions, ...).

- The use of the most sophisticated calculational methods in neutronics so that the (E-C) values be exactly representative of the quality of the nuclear data;

That's the reason why the conclusions are derived from an adjustment involving all types of integral data (fast, thermal, transmission, ...).

- Establishment of covariance matrices.

Since there are no covariance matrices in JEF2 (except for ^{238}U and ^{239}Pu), covariances have been generated on the basis of personal judgement assuming medium range correlations.

OPERATION OF THE STATISTICAL ADJUSTMENT METHOD

The main objective in nuclear data adjustment is to check the consistency of integral and microscopic data so as to create a data set able to calculate any integral parameter with the best reliability and with an accuracy equal to that of the measurements.

In other words one has to consider not only the accuracy of the adjusted microscopic data, but also the accuracy of the corrected integral data.

In the adjustment not only the vectors of the integral and microscopic data are changed but also the related covariances matrices. These changes are optimized changes if certain conditions are fulfilled :

- When assuming Gaussian distribution of the errors, the theory imposes to the a posteriori χ^2 value the relationship $\chi^2 = N \pm \sqrt{2N}$ (1), that is the condition for the microscopic and integral data to be consistent. If this relationship is not satisfied, all the uncertainties have to be multiplied by the enhancement factor $\left(\frac{\chi^2}{N}\right)^{1/2} = E.F.$

- The cross-section modifications have to be small to satisfy the linearity principle, i.e, to be consistent with the calculation of the sensitivity coefficients that is generally performed using Generalized Perturbation Theory.

These constraints have been guidances for the operation of the adjustment method.

In a first step, the integral data of each experimental program have been analyzed separately in order to check their internal consistency. Strict consistency was obtained in very few cases. Personal judgement was used to declare the data as consistent or not, but in general the data were kept when the chi-squired per degree of freedom values $\left(\frac{\chi^2}{N}\right)$ were less than 3 or 4. In that way 16 data were eliminated. Another way to get consistency is to enlarge the a priori variances of the microscopic data.

It has been shown [3] that very sophisticated covariance matrices characterized by small variances couldn't have any practical use because of the imperfect consistency of the integral data for reasons of experimental technique or calculational method. This also has been a guidance to establish the covariance matrices for the JEF2 evaluations.

In the final adjustment the retained (selected) integral data were put together. Here again the data originating too high χ^2 values were eliminated on the argument of inconsistency with the whole of the integral information. 26 additional integral data were eliminated, making a total of 42 out of 169.

As a matter of fact, the condition (1) written also as : $\frac{\chi^2}{N} = 1 \pm \sqrt{\frac{2}{N}}$ has to be strictly respected. The figure 1 shows the adjustments obtained with $\frac{\chi^2}{N} = 3.15$ (N=169), with $\frac{\chi^2}{N} = 1.64$ (N=132), and $\frac{\chi^2}{N} = 1.07$ (N=127).

The adjustment with $\frac{\chi^2}{N} = 1.07$ is different from the other ones and has to be preferred : The "truth" between 1 keV and 100 keV is closely known because of the work of the subgroup 5 of the international cooperation on evaluation. The adjusted cross-section related to $\frac{\chi^2}{N} = 1.07$ is very consistent with WESTON's renormalized data [4].

On the contrary there are nuclei for which the adjustments are rather insensitive to the $\frac{\chi^2}{N}$ value such as ^{238}U, ^{56}Fe, ^{23}Na, ^{16}O, ...

When dealing with data adjustments one has sometimes to face situations of multi-minima, i.e, situations for which very similar XH12 values per degree of freedom correspond to significantly different adjustments. This means that the XH12 criterion is necessary but may be not sufficient to characterize a situation of a generalized minimum.

For this type of situation the preferable situation is the one which simultaneously improves the "a posteriori" accuracy for all integral parameters. The solution which looks obvious has also the merit of being consistent with the primary objective of the nuclear data adjustment.

The nuclear parameters concerned by the adjustments are :

ν, σ_f, $\sigma_{n,n}^{removal}$, $\sigma_{n,n'}^{removal}$, $\sigma_{capture}$ for the following (17) nuclei : ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{238}U, ^{235}U, Zr, ^{56}Fe, ^{58}Ni, ^{52}Cr, ^{27}Al, Gd, ^{23}Na, ^{16}O, ^{12}C, ^{10}B, "H_2O".

RESULTS OBTAINED WITH 127 SELECTED INTEGRAL DATA

127 integral data are few with respect to the large number of nuclear group data ($\leq$ 1275) to be adjusted, but the technique of LAGRANGE multipliers helps in managing such a situation. Nevertheless the present integral data base is complete in that sense it contains the needed types of information affecting all the nuclear parameters in the whole energy range.

The results are listed in the Table 1, but the main features of the adjustments are summarized in what follows :

- ^{239}Pu
  Significant decrease (10 %) of $\sigma_{n,n}$ above 100 keV.
  This statement is consistent with the conclusions derived from the work of the subgroup 5 of the international cooperation on Evaluation.

- ^{240}Pu
  - Decrease (~ 10 % - 15 %) of σ_f in the threshold region.
  - Significant (~ 8 %) decrease of σ_c above the keV region.

- ^{241}Pu
  - Slight increase of σ_f above 2 MeV.

- ^{242}Pu
  - Trend for an increase of σ_f.
  - Significant (~ 10 %) decrease of σ_c.

- ^{238}U
  - Increase (10 %) of $\sigma_{n,n}$ above 6 MeV.
  - Trend to decrease σ_c between 500 eV and 10 keV.

- ^{235}U
  - General trend to decrease $\sigma_{n,n}$ between 25 keV and 2 MeV by a few %.
  - Significant increase of σ_c in the eV and keV region. Significant decrease above ~ 500 keV.

- ^{56}Fe
  - ♦ Significant decrease (~ 15 %) of $\sigma_{n,n}$, below 15 MeV, increase above 6 MeV.
  - ♦ General trend to decrease σ_c.
  - ♦ Trend to decrease σ_t below 6 MeV.

- ^{58}Ni
  - ♦ Important decrease of σ_c to be understood as absorption cross section, $\sigma_{(n,p)}$ might be implied (problem of Q value ?).

- ^{23}Na
  - ♦ Strong decrease of $\sigma_{n,n'}^{removal}$.

- ^{16}O
  - ♦ Significant increase of $\sigma_{n,n'}^{removal}$.
  - ♦ Significant decrease of $\sigma_{n,n'}^{removal}$ (~ 15 %) below the 1st resonance in the energy region where $\bar{\mu}$ is negative. Being given the quality of the fit of $\sigma_{n,n}$ into the experimental data, it is suggested that the origin of the discrepancy could be the angular distribution.

- ^{12}C
  Nice.

- ^{10}B
  Nice.

COMMENTS

In this first approach all the considered nuclear parameters have been considered as free. Improvements are needed, in particular the constraint of a constant total cross section should be introduced. The difficulty is in the fact that σ_t plays a role in neutronic via the so called transport cross section $\sigma_{tr} = \sigma_t - \mu\, \sigma_{n,n}$. If σ_{tr} is introduced in the adjustment procedure, covariance matrices have to be established for it and the adjustment has to be split between σ_t, $\sigma_{n,n}$ and the angular distributions (Difficulties !).

Another question is about the discrepancies insufficiently reducible by adjustment. Is it due to the data (non linearity in the adjustment ; this is obvious for some nuclei), to insufficient quality of the calculational methods concerning in particular the treatment of the slowing down and of the leakages in the cell code ?

If one plots the "a posteriori" $\frac{E-C}{C}$ values as a function of the Buckling (greater is B^2, greater are the leakages) (see figure 2), one doesn't see any systematic effect, except a correlation between experiments loaded with Oxygen (Z2, ZONA2, ZOCO1, ...). This correlation appears (figure 3) also if the same $\frac{E-C}{C}$ values are plotted as a function of the spectral hardness parameter r $\left(r = \frac{< \nu\Sigma_f >}{< \xi\Sigma_s >} \right)$.

One concludes that there is no obvious deficience in the calculational method but a data problem (essentially Na and O) that is energy dependent.

CONCLUSIONS

The benchmarking of JEF2 is progressing satisfactorily. Contributions have been given from almost all the European Laboratories : WÜRENLINGEN, WINFRITH, BOLOGNA, SACLAY, CADARACHE. It is still not complete and in particular more information is needed to know more about the exact value of nuclei of the general purpose file such as ^{240}Pu, ^{242}Pu, at high energy, Cr, Zr, Gd, Al, ...

Almost everything remains to be done for what concerns the minor Actinides especially those involved in transmutation studies, the F.P's. That's the task for the coming years.

JEF2.2 appears as a good file, since it calculates the K_{eff} of most fast systems with a discrepancy of the order of 1200 pcm and the thermal with a discrepancy still less (800 to 1000 pcm). When the discrepancies are greater it is due to the conjunction of a data problem and of a calculational method. Concerning the spectral indices the discrepancies are greater but compatible with the experimental uncertainties.

The information obtained in these last 6 months are sufficiently reliable to suggest a first program of revision of evaluations.

The observed deficiencies concern only one parameter often on a limited portion of energy, very rarely for the whole energy range but the consequences on Integral parameter calculation are severe.

This is the merit of a generalized benchmarking involving all the data types covering a large energy range to reveal these local needs for improvement. With that respect it is highly desirable to include in JEF2 validation, a set of benchmarks designed for fusion.

The importance of the parameter $\frac{\chi^2}{N}$ should be stressed again. It is the guarantee of a good adjustment with physical meaning. It has revealed that a non negligible proportion of integral data are inadequate for data validation purpose. The most interesting of them should be reanalysed.

ACKNOWLEDGEMENTS

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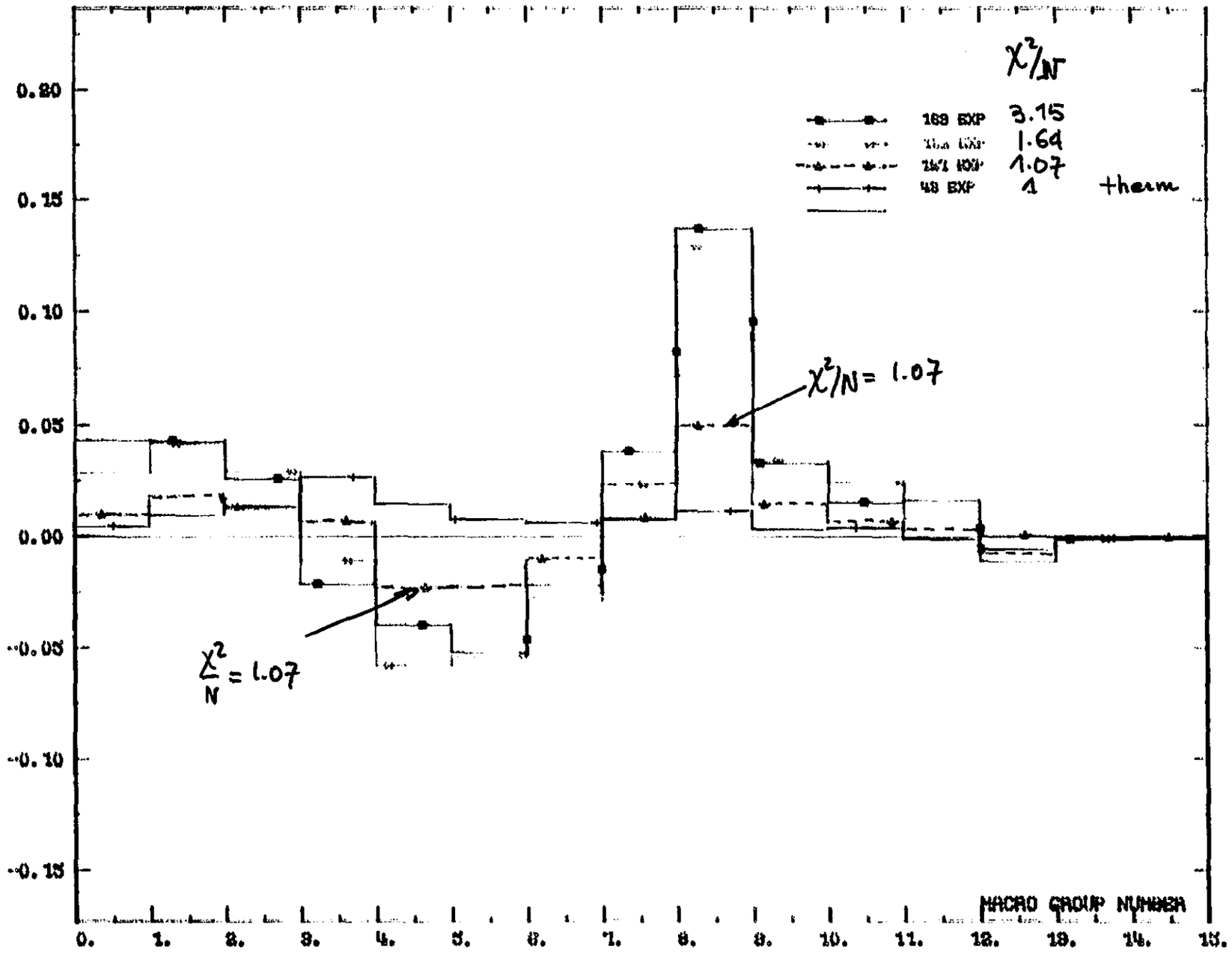
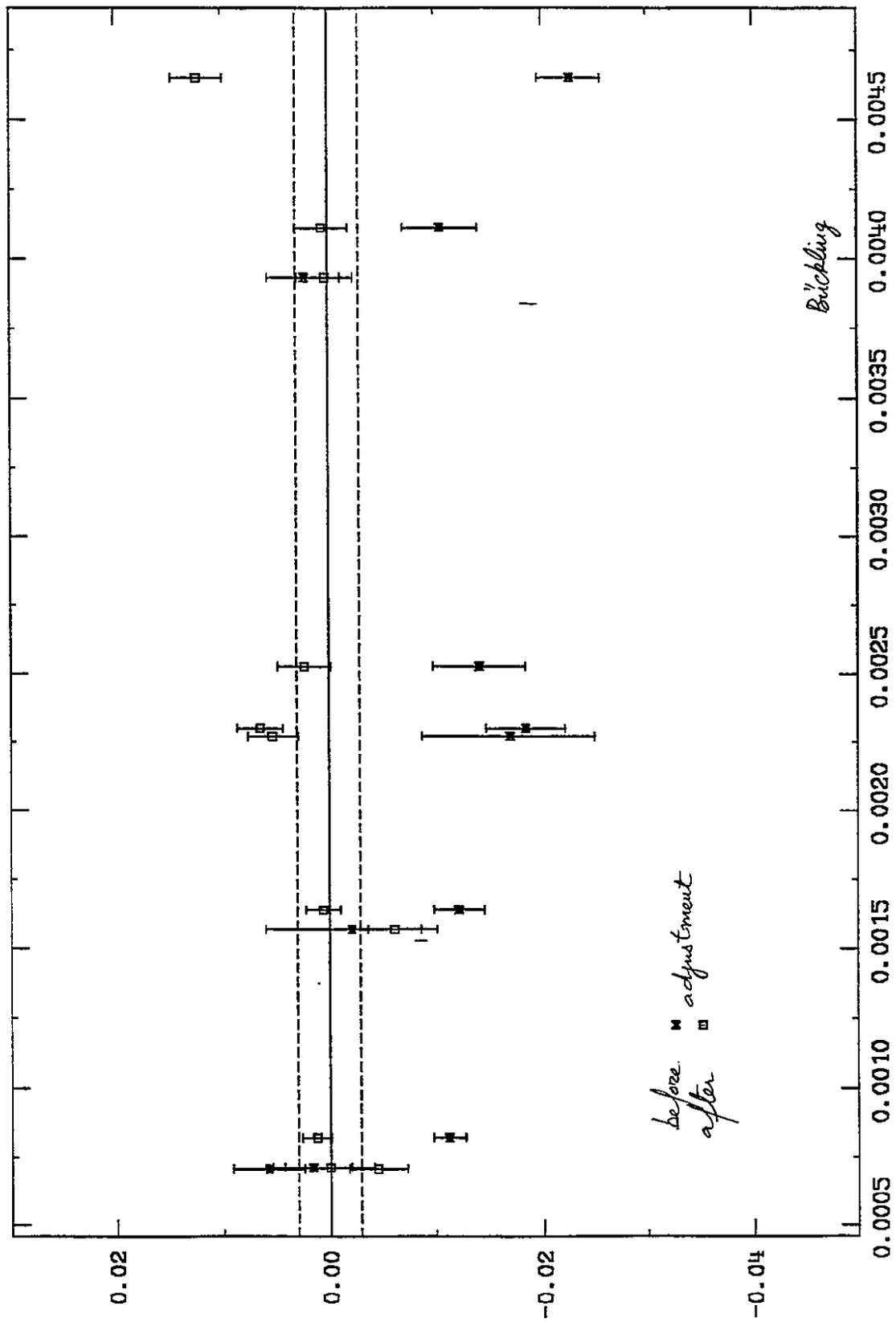
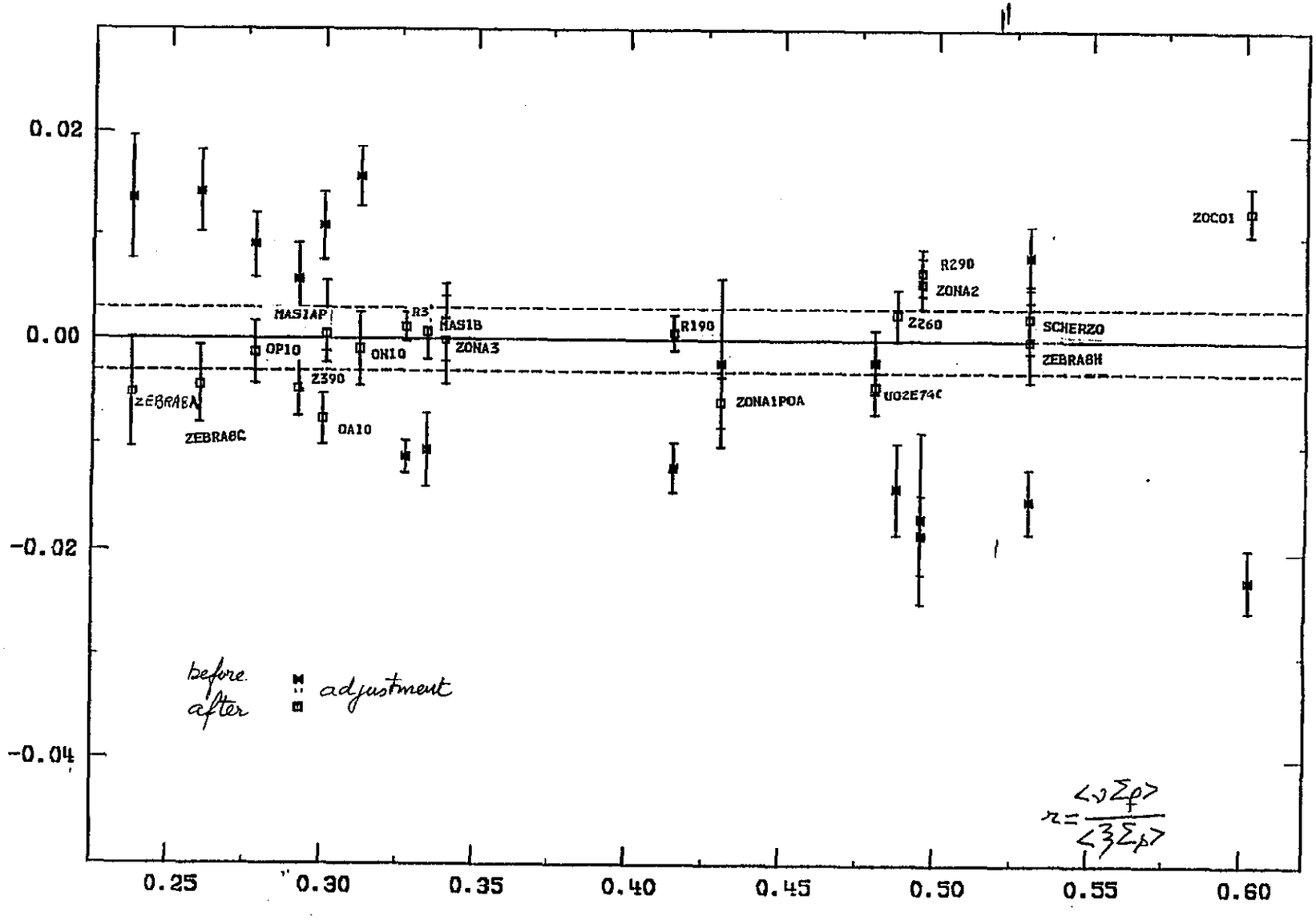


FIGURE 1

FIGURE 2

"A posteriori" $\frac{E-C}{C}$ *K_{eff} values versus the Buckling data*





"A posteriori" $\frac{E-C}{C}$ K_{eff} values versus the r parameter data

FIGURE 3