FR8700183

COMMISSARIAT A L'ENERGIE ATOMIQUE

CENTRE D'ETUDES NUCLEAIRES DE SACLAY
Service de Documentation
F91191 GIF SUR YVETTE CEDEX

CEA-CONF-- 8718

R5

UNRESOLVED RESONANCE SELF SHIELDING CALCULATION : CAUSES AND IMPORTANCE OF DISCREPANCIES

RIBON, P.; TELLIER, H. CEA CEN Saclay, 91-Gif-sur-Yvette (France). IRDI

Communication présentée à : Meeting on advances in reactor physics and safety
Saratoga Springs, NY (USA)
17-19 Sep 1986

UNRESOLVED RESONANCE SELF SHIELDING CALCULATION: CAUSES AND IMPORTANCE OF DISCREPANCIES

P. RIBON and H. TELLIER

Service d'Etudes de Réacteurs et de Mathématiques Appliquées
Centre d'Etudes Nucléaires de SACLAY - 91191 - FRANCE

ABSTRACT

To compute the self shielding coefficient, it is necessaryto know the point-wise cross-sections. In the unresolved resonance region, we do not know the parameters of each level but only the average parameters. Therefore we simulate the point-wise cross-section by random sampling of the energy levels and resonance parameters with respect to the Wigner law and the x^2 distributions, and by computing the cross-section in the same way as in the resolved regions. The result of this statistical calculation obviously depends on the initial parameters but also on the method of sampling, on the formalism which is used to compute the cross-section or on the weighting neutron flux. In this paper, we will survey the main phenomena which can induce discrepancies in self shielding computations. Results are given for typical dilutions which occur in nuclear reactors.

I. INTRODUCTION

It is not possible for reactor calculation to use a very fine description of the neutron cross-sections in the resonance energy range. It would be too computer time consuming. Therefore, the reactor physicists use the concept of multigroup self shielded cross-section. This concept takes into account the fine structure of the actual cross-sections and the concentration of the resonant nuclide in the multiplying medium. This concentration is introduced by a background cross-section. The ratio between the self shielded cross-section and the average cross-section is called the self shielding factor. With the new advanced reactor (large fast breeder or tight pitch water reactor) the importance of the resonance energy range increases. So, it becomes necessary to compute this self shielding factor with great accuracy. Recently a benchmark exercise was carried out on behalf of the Nuclear Energy Agency. Several laboratories answered this exercise. The various results are significantly different [1]. Therefore, it seemed interesting to make a systematic study of the different effects which can induce discrepancies in self shielding calculations. In addition to the problem of numerical accuracy which can occur in the calculations, four different sources of discrepancies had been recorded. They are: the basic data themselves, the sampling methods, the nuclear processing to obtain the point-wise cross-sections (extra resonances, multilevel formalism) and the neutron processing to generate the multigroup cross-sections (Bondarenko or slowing down flux weighting). We have studied these effects in the case of the ^{238}U unresolved resonance region between 3.35 and 37.0 keV. This energy range is divided into six groups corresponding to the usual energy mesh of the APOLLO thermal neutron reactor calculation code [2]. The computations of cross-sections and self shielding factor are performed for the mean energy of each group and an energy range equal to 800 eV.

II. NUMERICAL ACCURACY

As we wish to evaluate differential effects in calculation, it is necessary, first of all, to check carefully if the accuracy of the numerical calculation is sufficient to obtain a meaningful difference. To compute the average cross-sections and the self shielding factors, it is necessary to reconstruct a point-wise cross-section with the resonance parameters and to do an integration. The accuracy of the result depends on the number of energy points where the cross-section is computed. To generate the energy mesh, we use a formalism which has several levels of accuracy [3]. Between two levels the number of points is approximatively increased by a factor $\sqrt{2}$. The user can choose the level of accuracy. A set of calculations with several accuracy levels and an extrapolation with Pade's method can be used to verify the accuracy of the numerical computation. An example is given in Table I for an energy equal to 20.7 keV. The relative difference between the extrapolated value and the value obtained with level 2 is of the order of 10^{-5} for the cross-section and 10^{-6} for the self shielding factor. Therefore we can make further calculations with accuracy level 2, the relative difference between two different computations will be significant.

TABLE I

Numerical Accuracy Check

E = 20.7 keV					
Accuracy	Number of points	$\langle \sigma_s \rangle$	f_s(50 b)	$\langle \sigma_\gamma \rangle$	f_γ(50 b)
Level 1	742	13.3487	0.921853	0.564985	0.970431
Level 2	1062	13.3485	0.921834	0.564898	0.970432
Level 3	1480	13.3484	0.921833	0.564900	0.970433
Extrapolation	-	13.3483	0.921833	0.564900	0.970433

III. INFLUENCE OF BASIC DATA

There are several ^{238}U evaluated files which can be used for reactor calculations by various laboratories. These evaluated files may recommend basic neutron data (level spacing, average resonance parameters or strength function) which are slightly different. To check the influence of the input neutron parameters, we performed self shielding calculations with the four last available files: ENDF/B4 (1973), KEDAK (1975), ENDF/B5 (1979) and JEF-1 (1979).

The average parameters which are used in these files are compared in Table II. The most important differences are observed for the strength functions. This will induce significant disagreements in the calculation of the scattering cross-sections.

TABLE II

Average parameters of the evaluated files

	ENDF/B4	KEDAK	ENDF/B5	JEF-1
$R'(10^{-13}$ cm)	0.9184	0.9440	0.9184	0.9360
D_o (eV)	19.98	20.40	20.00	19.80
Γ_γ (meV)	23.5	23.5	23.5	23.5
$10^4.S_0$	1.05	1.16	1.05	0.85
$10^4.S_1$	1.57	1.99	1.045	1.41

To compute the cross-sections, we use a formalism which takes into account the scattering interference between resonances and a single level Breit and Wigner formula for the capture cross-section. The interference term between resonances is [4]:

$$\sum_{\lambda,\lambda' \neq \lambda} \frac{\Gamma n_\lambda \, \Gamma n_{\lambda'}}{\Gamma_\lambda \, \Gamma_{\lambda'}} \left(\cos 2\phi \, \frac{xx'-1}{(1+x^2)(1+x'^2)} - \sin 2\phi \, \frac{x+x'}{(1+x^2)(1+x'^2)} \right)$$

It is slightly differentfrom the usual multilevel Breit and Wigner formalism. This formalism was checked relative to an exact multilevel formalism. The difference is very small for the energies which are involved in this work. This formalism allows Doppler broadening by analytical calculations which are more economical of computer time.

The self shielding calculations are performed with the narrow resonance approximation. The effective cross-sections are given by the Bondarenko model

$$\sigma_{x,eff} = \frac{\int \varphi(E) \, \sigma_x(E) dE}{\int \varphi(E) dE}$$

with the fine structure flux

$$\varphi(E) = \frac{E^\alpha}{\sigma_t(E) + \sigma_d}$$

σ_x is the partial cross-section, σ_t the total cross-section and σ_d the background cross-section. The self shielding factor is

$$f_x = \frac{\sigma_{x,eff}}{\sigma_{x,\infty}}$$

The calculations are done for a temperature equal to 300 K with $\alpha = -1$. The given results are the average of four statistical samples. The values of the cross-sections and the statistical errors are given in Table III for the scattering and in Table IV for the capture. They present an important spread. The actual dispersion between evaluations was calculated by quadratic substraction of the statistical error from the apparent dispersion. It is about 5 to 6 percent for scattering and 6 to 8 per cent for capture, an order of magnitude higher than the statistical error. The lower values are obtained with JEF-1 and the higher ones with KEDAK.

TABLE III

Influence of basic data on scattering cross-section

Energy / File	5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
ENDF/B4	15.447 ±0.367	14.463 ±0.036	13.910 ±0.107	13.297 ±0.095
KEDAK	16.277 ±0.195	15.602 ±0.141	14.774 ±0.105	14.154 ±0.071
ENDF/B5	16.460 ±0.160	15.522 ±0.092	14.936 ±0.105	14.317 ±0.125
JEF-1	14.647 ±0.058	14.735 ±0.072	14.386 ±0.100	12.986 ±0.047
Average value	15.708	14.831	14.252	13.689
Dispersion	0.833	0.896	0.792	0.648

TABLE IV

Influence of basic data on capture cross-section

Energy / File	5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
ENDF/B4	0.8928 ±0.0096	0.7538 ±0.0100	0.6462 ±0.0046	0.5531 ±0.0039
KEDAK	0.9772 ±0.0041	0.8440 ±0.0058	0.7205 ±0.0029	0.6081 ±0.0064
ENDF/B5	0.8524 ±0.0027	0.7349 ±0.0096	0.6120 ±0.0042	0.5522 ±0.0037
JEF-1	0.8209 ±0.0107	0.6846 ±0.0076	0.6013 ±0.0026	0.5435 ±0.0025
Average value	0.8858	0.7543	0.6450	0.5642
Dispersion	0.0677	0.0665	0.0539	0.0296

TABLE V

Influence of basic data on scattering self shielding factor (σ_d = 50 b)

Energy / File	5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
ENDF/B4	0.8674 ±0.0066	0.9092 ±0.0022	0.9310 ±0.0069	0.9625 ±0.0014
KEDAK	0.8602 ±0.0053	0.9026 ±0.0025	0.9324 ±0.0044	0.9541 ±0.0034
ENDF/B5	0.8785 ±0.0047	0.9176 ±0.0010	0.9431 ±0.0044	0.9638 ±0.0020
JEF-1	0.9061 ±0.0032	0.9400 ±0.0015	0.9588 ±0.0013	0.9723 ±0.0011
Average value	0.8781	0.9174	0.9413	0.9632
Dispersion	0.0202	0.0163	0.0128	0.0074

TABLE VI

Influence of basic data on capture self shielding factor (σ_d = 50 b)

Energy / File	5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
ENDF/B4	0.8666 ±0.0029	0.9142 ±0.0037	0.9460 ±0.0009	0.9678 ±0.0013
KEDAK	0.8713 ±0.0015	0.9242 ±0.0040	0.9522 ±0.0017	0.9662 ±0.0026
ENDF/B5	0.8686 ±0.0030	0.9195 ±0.0026	0.9934 ±0.0016	0.9726 ±0.0013
JEF-1	0.8739 ±0.0008	0.9261 ±0.0013	0.9510 ±0.0018	0.9721 ±0.0021
Average value	0.8701	0.9210	0.9807	0.9697
Dispersion	0.0032	0.0053	0.0033	0.0032

The self shielding factors are also different according to the file. But the differences are smaller than in the case of the cross-sections and they are in the opposite direction. The dispersion varies from 2 to 1 percent versus energy for scattering. It is about 0.4 percent for capture. But the observed differences on the effective cross-sections (product $f_x * \sigma_{x,\infty}$) remain important and can have non negligible effects in reactor calculations. The higher values of f are obtained with JEF-1 and the lower ones for ENDF/B4. The variations of f_x as a function of the background cross-section are displayed for these two files on figure 1 for the scattering and figure 2 for capture. As an example of the detailed results, Table V gives the self shielding factor, the statistical error, and the dispersion for σ_d = 50 barns in the case of scattering, Table VI gives the analogousresults for capture.

IV. INFLUENCE OF SAMPLING METHODS

To compute the self shielding in the unresolved resonance energy region, where we only know the average resonance parameters, the usual method is to generate one or several resonance ladders and to process them in the same way as the resolved resonances. These ladders are generated by the Monte-Carlo method with respect to the Porter and Thomas law for the neutron widths and the Wigner law for the resonance spacings. The main difficulty of this technique is to reduce the dispersion of the data and results. The basic method to improve the statistics and to reduce the dispersion is to generate a great number of samples and to average the results. This technique can be considered as a reference but it is too computer time consuming for routine calculations. There are several methods to improve the accuracy of the cross-section calculation in the unresolved resonance energy range, both for Γn_λ and E_λ. One of these seems to be very efficient. The distribution of the resonance energies is given by a set of random matrix eigenvalues. The neutron widths are obtained by a regularized sampling method [5]. In this method, if we want to obtain N values of the neutron width, the integral probability range (0,1) is divided into N subintervals (0, 1/N), (1/N, 2/N)... and a random number P_i is generated in each subinterval. This number P_i determines x_i in this interval. It can be shown that the average value of any function F(x), calculated from this sample is unbiased and that the dispersion is greatly reduced.

We have compared the regularized method with the usual random method in the case of ENDF/B4. The average results of 16 samples are given in Table VII for scattering and Table VIII for capture (average cross-section and self shielding factor for σ_d = 50 barns). From the statistical point of view, the average values do not present any significant difference but the dispersion is reduced by a factor 2 or 3 when we use the regularized samples.

V. INFLUENCE OF THE NUCLEAR PROCESSING

Even if they use the same average parameters, the results of self shielding calculations can be slightly different according to the computer code. All the computer codes do not use the same same nuclear formalism. They can take into account, or not, the interference between resonances, the influence of the resonances which are located outside the sample or the effect of the large "s" wave resonances which can be resolved in the low energy part of the unresolved region. In this section, we will examine the magnitude of these effects.

TABLE VII

Influence of sampling method on scattering

Energy		5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
σ_∞	Random	14.993 ±0.233	14.045 ±0.208	13.693 ±0.118	13.555 ±0.153
	Regularized	15.396 ±0.123	14.511 ±0.075	13.908 ±0.059	13.402 ±0.052
f_{50}	Random	0.8736 ±0.0075	0.9193 ±0.0061	0.9414 ±0.0040	0.9570 ±0.0033
	Regularized	0.8659 ±0.0037	0.9060 ±0.0020	0.9343 ±0.0021	0.9586 ±0.0009

TABLE VIII

Influence of sampling method on capture

Energy		5.0-7.5 keV	7.5-11.1 keV	11.1-16.6 keV	16.6-24.8 keV
σ_∞	Random	0.8713 ±0.0180	0.7443 ±0.0124	0.6443 ±0.0084	0.5494 ±0.0101
	Regularized	0.8954 ±0.0047	0.7486 ±0.0037	0.6548 ±0.0025	0.5595 ±0.0021
f_{50}	Random	0.8705 ±0.0029	0.9190 ±0.0038	0.9510 ±0.0010	0.9690 ±0.0016
	Regularized	0.8700 ±0.0017	0.9149 ±0.0016	0.9490 ±0.0011	0.9691 ±0.0007

V.1. Multilevel effect

If we consider a large number of resonances, there are compensations between the positive effects and the negative effects of the interference. Therefore the average cross-section is not affected. But the point-wise cross-section is modified. Then the effective cross-section and the self-shielding factor are changed. We know that in the case of the low energy resonances of uranium 238 the multilevel effect on capture is of the order of one per cent for a 50 barn dilution [6]. For the resolved resonance region, this effect decreases when the energy of the resonances increases. For the unresolved resonance region, we performed two self-shielding calculations, one with a single level Breit and

Wigner formula and the other with interference in the scattering cross-section. We observed a very slight difference. The effective integral decreases when we use a multilevel formalism. As the effect does not seem to depend on the energy we can take an average over all the energy range. The relative difference between the self-shielding factor computed with a multilevel formalism and the same factor calculated with a single level formalism is given in Table IX.

TABLE IX

Influence of multilevel formalism averaged on whole energy

Dilution (barn)		10	50	200
$\frac{f_{ML} - f_{SL}}{f_{SL}}$ (10^{-2})	scattering	0.28 ± 0.13	0.13 ± 0.06	0.06 ± 0.03
	capture	0.07 ± 0.05	0.08 ± 0.03	0.02 ± 0.02

V.2. Influence of resolved resonances

Below 6 keV, the large "s" wave resonances of ^{238}U are resolved. Only the small "s" wave resonances and the "p" wave resonances are not resolved. If we consider, for self shielding calculations, that all the resonances are unresolved, we may increase the statistical fluctuations. To check the effect of the large resolved resonances, we have used the following method. Starting from a reference case which is the average of 16 statistically independent samples, we have performed two other calculations with 16 samples which are not independent. In the first calculation, the four largest resonances are the same for all the samples, in the second calculation the eight largest resonances are common to all the samples. So we simulate the effect of 4 or 8 resolved resonances. The results on the self shielding factor and its dispersion are given in Table X for the 5.0-7.5 keV range and a 50 barn dilution. The mean value remains unchanged but the dispersion is greatly improved for the scattering. No effect is observed for the capture.

TABLE X

Effect of resolved resonances on self shielding factor

$5.0 < E < 7.5$ keV $\sigma_d = 50$ b	*Scattering*	*Capture*
Reference	0.8652 ± 0.0148	0.8691 ± 0.0061
4 resolved resonances	0.8512 ± 0.0016	0.8682 ± 0.0055
8 resolved resonances	0.8509 ± 0.0011	0.8705 ± 0.0073

V.3. Remote resonance effect

Because of the interference effects, the cross-section inside an energy interval (E_M, E_m) depends on the resonances which are located outside this interval. Thus the self shielding factor may be different if we take into account these remote resonances or not. Two computations allowed us to calculate this influence. The reference computation of the self shielding factor is performed with remote resonances for all the energies above E_M and below E_m. These resonances intervene by their average contribution. In the second calculation, only the resonances located inside the interval (E_M/α,E_m) are taken into account.. Then there is a slight asymetry. When we do not take into account the remote resonances, the self shielding factor decreases slightly. No shift can be observed when the energy increases. Table XI gives the relative decrease of the self shielding factor for the energy range 3.35-37 keV in unit 10^{-2}.

TABLE XI

Influence of the remote resonances for the energy range 3.35-37 keV

Dilution	10 b	50 b	100 b
Scattering	- 0.08	- 0.035	- 0.013
Capture	- 0.025	- 0.006	- 0.001

The effect is not important. It is smaller for capture than for scattering and it decreases with dilution.

VI. INFLUENCE OF THE NEUTRON PROCESSING

At low energy the ^{238}U resonances are neither narrow nor wide. A slowing down calculation of the flux is necessary to compute the self shielding factor. At high energy the resonances become narrow and the narrow resonance approximation is sufficient. We determined the influence of the flux calculation method in the unresolved resonance energy range by performing two different computations, the first one with a slowing down flux (f_{SD}) and the second with the narrow resonance approximation (f_{NR}). These calculations were performed as a function of energy and background cross-section in the case of four statistically independent samples. Table XII gives the results of the ratio f_{SD}/f_{NR} for scattering and Table XIII for capture.

TABLE XII

Influence of slowing down on scattering self shielding factor $f_{SD}/f_{NR} - 1$ in unit 10^{-2}

Energy / Dilution	3.35-5 keV	5.0-7.5 keV	7.5-11.1 keV	11.1-37 keV
10 b	-0.01 $\pm$ 0.54	-0.03 $\pm$ 0.23	0. $\pm$ 0.03	0. $\pm$ 0.04
50 b	+0.07 $\pm$ 0.30	+0.02 $\pm$ 0.12	+ 0.01 $\pm$ 0.04	+ 0.01 $\pm$ 0.01
200 b	+0.07 $\pm$ 0.15	+0.03 $\pm$ 0.06	+ 0.01 $\pm$ 0.02	+ 0.02 $\pm$ 0.02

TABLE XIII

Influence of slowing down on capture self shielding factor: $f_{SD}/f_{NR} - 1$ in unit 10^{-2}

Energy / Dilution	3.35-5 keV	5.0-7.5 keV	7.5-11.1 keV	11.1-37 keV
10 b	-0.51 ± 0.33	-0.35 ± 0.26	0.27 ± 0.19	0.06 ± 0.12
50 b	+0.43 ± 0.23	+0.27 ± 0.16	+ 0.17 ± 0.13	+ 0.05 ± 0.08
200 b	+0.19 ± 0.11	+0.12 ± 0.08	+ 0.08 ± 0.07	+ 0.04 ± 0.03

The slowing down process does not seem to affect the scattering self shielding. But there is an effect on the capture self shielding. This effect is small but significant essentially for low dilutions (see figure 3). This effect decreases with energy and dilution. Nevertheless it is recommended to take into account the slowing down up to 7.5 keV.

VII. CONCLUSION

Several assumptions and approximations can affect the computation of the self shielding factor in the unresolved resonance energy range. These various effects have been studied in the case of uranium 238 in the energy range 3.35-37 keV. Some of these assumptions can significantly modify the values of the self shielding factors (with the exception of the basic data, the effect remains small). Others can only influence the dispersion that is to say the accuracy of the calculation. The main conclusions are summarized in Table XIV.

TABLE XIV

Influence / Effect	Strong modification of f	Small modification of f	Improvement of the accuracy
Basic Data	*		
Sampling method			*
Resolved resonances			*
Remote resonances		*	
Multilevel formalism		*	
Slowing down		*	

All these effects do not seem to explain the discrepancies which are observed in the Nuclear Energy Agency benchmark. The energy range which we proposed in the benchmark (2.0-3.3 keV) is lower than the energy range which is studied in this work and the different effects can be slightly higher. Nevertheless we think that they are too small to explain the spread of the benchmark results which give $\sigma_{c\infty}$ values from 1.107 b (MICROS Code) to 1.080 b (TIMS Code) and

self-shielding factors for a 10 b background cross section between 0.403 and 0.449, that is to say a difference by 7%. Our results for the same energy range are respectively 1.095 b and 0.412 [7].

To do an accurate calculation of the self shielded cross-section, we recommend taking into account the remote resonances, using a multilevel formalism, and doing a slowing down calculation mainly for the lower part of the unresolved resonance energy range. All this can be performed with only a very slight increase of computer time. To improve the accuracy of the calculation, we suggest the use of regularized sampling and taking into account the effect of the largest resonances which can be resolved. Up to now the format of the evaluated files does not allow the application of this last technique. It would be necessary to increase the informations presently included in the evaluated files. As a matter of fact, the knowledge of the average parameters is not sufficient to provide an accurate description of the cross-section behaviour. Several propositions have already been made to improve the content of the files. One of these is to specify the infinite dilution cross-section and the shielding factors $f_x(0)$ for a zero background cross-section together with mean resonance parameters and statistical distributions [1]. The $f_x(0)$ factor can be obtained with a self indication measurement. Another proposition is that the best solution would be to incorporate in the files the point-wise cross-sections [8]. We support another method which is to introduce simultaneously the average parameters and the resolved parameters for the largest resonances. A threshold Γ^t on the neutron width for instance would indicate that all the resonances are assumed to be resolved for Γ_n larger than Γ^t while they would to be randomly generated for Γ_n smaller than Γ^t. It seems that this would imply only small modifications of the format but would lead to great improvement of the self shielding factor accuracy.

REFERENCES

[1] J.L. ROWLANDS: "Representation of unresolved resonance regions in evaluations and in calculation methods". Reactor Physics and shielding - Chicago, II, 516 (1984).

[2] A. KAVENOKY: "APOLLO, a general code for transport, slowing down and thermalization in heterogeneous media". Mathematical models and computational techniques for analysis of nuclear system. Ann. Arbor, CONF 730414, I, 95 (1973).

[3] N. CATSAROS: "Amélioration du calcul de l'effet Doppler pour des sections efficaces simple et multiniveau". CEA-N-2180 (1981).

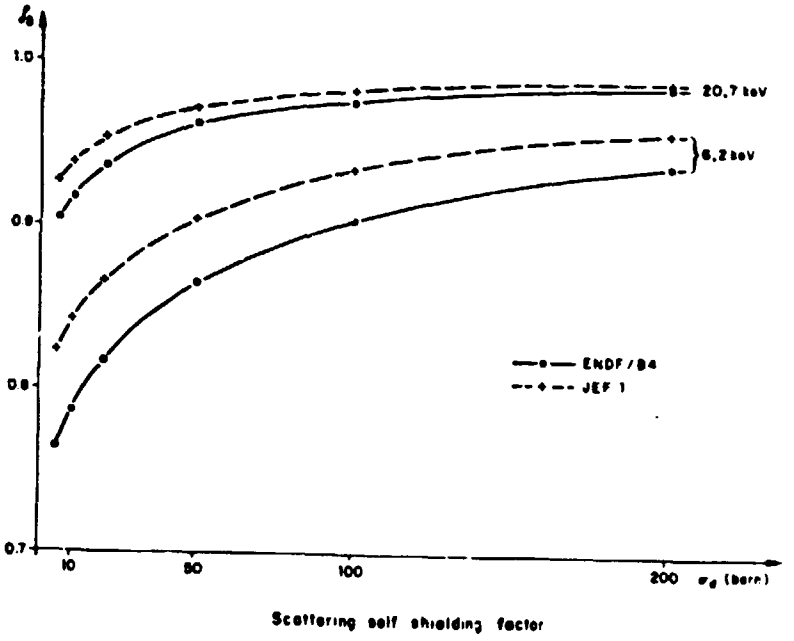
[4] P. RIBON et al.: Nuclear Data for Reactors - Paris 1966 - AIEA, I, 107 (1967).

[5] P. RIBON: Annals of Nuclear Energy 13, 209 (1986).

[6] H. TELLIER: Nuclear Science and Engineering 79, 393 (1981).

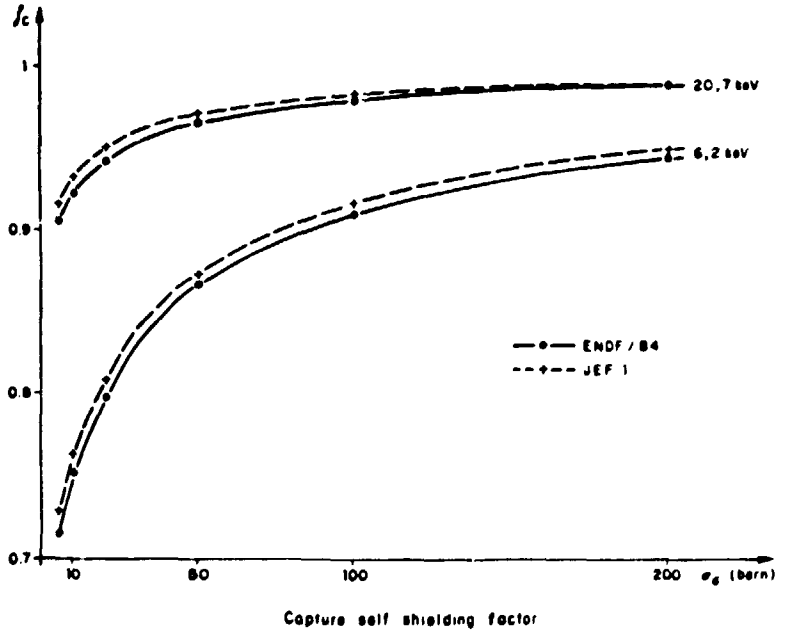
[7] P. RIBON et al.: "Etude des methodes de calcul de l'autoprotection dans les résonances" - CEA-N-2426 (1985).

[8] F. FROEHNER: Private Communication (1985).



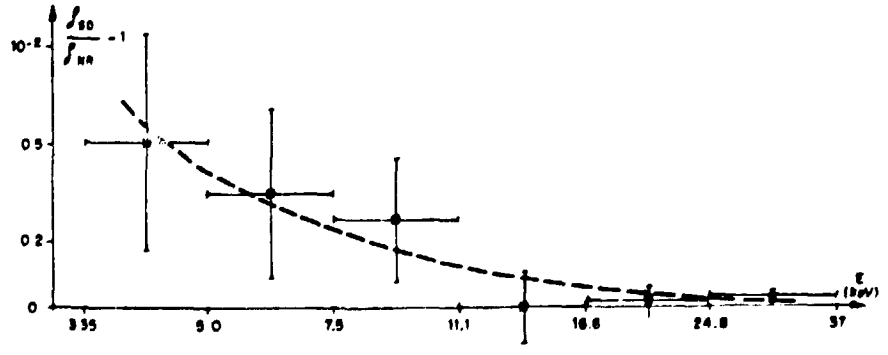
Scattering self shielding factor

Figure 1



Capture self shielding factor

Figure 2



Influence of slowing down
. σ_s = 10 barns

Figure 3