

International Evaluation Co-operation

VOLUME 15

**CROSS-SECTION FLUCTUATIONS
AND SELF-SHIELDING EFFECTS
IN THE UNRESOLVED RESONANCE REGION**

NUCLEAR ENERGY AGENCY

NEA/WPEC-15

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AND SELF-SHIELDING EFFECTS
IN THE UNRESOLVED RESONANCE REGION**

*A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee*

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FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The Working Party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The Parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries), and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report was issued by a Subgroup investigating self-shielding effects in the unresolved resonance region of structural materials. The objectives of the subgroup were to understand the effects of self-shielding above the resonance region on shielding and transport benchmark calculations, to determine the importance of a correct treatment of the effects, and to recommend procedures for representing the physics in this region in a manner consistent with processing code capabilities.

The opinions expressed in this report are those of the authors only and do not represent the position of any Member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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SUMMARY

NEA/NSC Subgroup 15 has had the task to assess self-shielding effects in the unresolved resonance range of structural materials, in particular their importance at various energies, and possible ways to deal with them in shielding and activation work. The principal results achieved are summarised briefly, in particular:

- *New data base consisting of high-resolution transmission data measured at Oak Ridge and Geel;*
- *Improved theoretical understanding of cross-section fluctuations, including their prediction, that has been derived from the Hauser-Feshbach theory;*
- *Benchmark results on the importance of self-shielding in iron at various energies;*
- *Consequences for information storage in evaluated nuclear data files;*
- *Practical utilisation of self-shielding information from evaluated files.*

Benchmark results as well as the Hauser-Feshbach theory show that self-shielding effects are important up to a 4-or 5-MeV neutron energy. Fluctuation factors extracted from high-resolution total cross-section data can be used to approximate also unmeasured fluctuations of partial cross-sections and their effects. More rigorous methods can be based on Monte Carlo sampling of resonance ladders provided that average resonance parameters are available. Needs for further work on techniques and codes have been identified but the Subgroup's main tasks appear to be fulfilled.

CROSS-SECTION FLUCTUATIONS AND SELF-SHIELDING EFFECTS IN THE UNRESOLVED RESONANCE REGION

1. The high-resolution transmission data

High-resolution transmission measurements performed on iron, nickel, chromium, titanium and, more recently on vanadium at Oak Ridge and Geel reveal strong resonance structure of the total cross-section which extends far into the so-called unresolved resonance region. For iron the boundary between the resolved resonance region (fully analysed, with all cross-sections parametrised in terms of resolved resonance parameters) and the unresolved resonance region (not parametrised by resonance analysis) is at about 0.86 MeV, which is the first inelastic threshold of ^{56}Fe . The resonance structure diminishes gradually as the energy grows but only above 4 MeV the observed relative fluctuations are smaller than 10%. As the resonance structures and ranges of analysed and non-analysed resonances are similar for all medium-weight structural materials, the results obtained for iron are also applicable to nickel, chromium, and vanadium. Therefore non-negligible self-shielding effects are expected up to about 3 to 5 MeV for all these elements.

A first question was raised: *Is the observed cross-section structure really the true resonance structure or is it affected by instrumental resolution and counting statistics?* In the Geel high-resolution transmission data measured with iron samples of 16-, 48- and 140-mm thickness by Berthold, Nazareth, Rohr and Weigmann (1994), it was easy to verify that above about 7 MeV most of the observed fluctuations were simply due to counting statistics (see Figure 1). From 7 MeV down to 4 MeV true fluctuations are seen but to some extent smoothed by limited instrumental resolution (see Figure 2). Monte Carlo simulations based on strength functions and effective radii of the various partial waves indicated that below 4 MeV most of the true structure was actually resolved (see Figure 3).

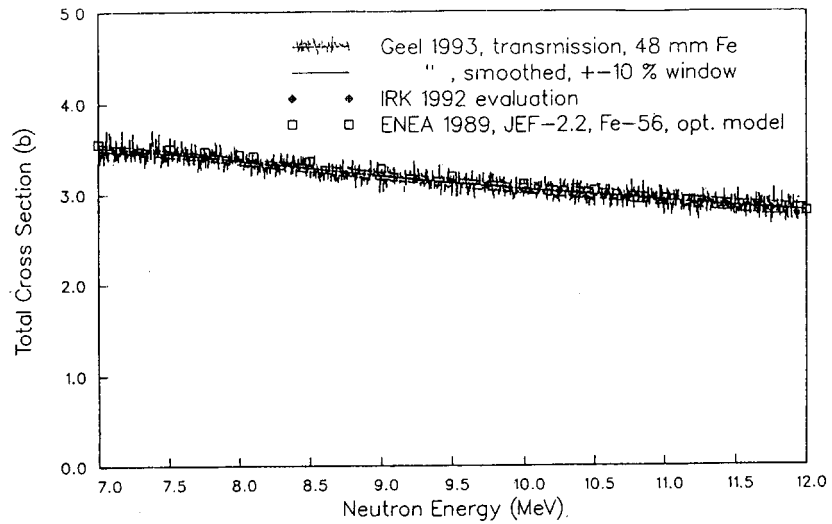


Figure 1

High-resolution total cross-section data for ^{56}Fe and smoothed energy-dependence with confidence band indicating standard uncertainty from counting statistics (Geel measurements): genuine fluctuations are drowned in noise from counting statistics above 7 MeV. IRK and JEF-2 (ENEA) evaluations are also shown.

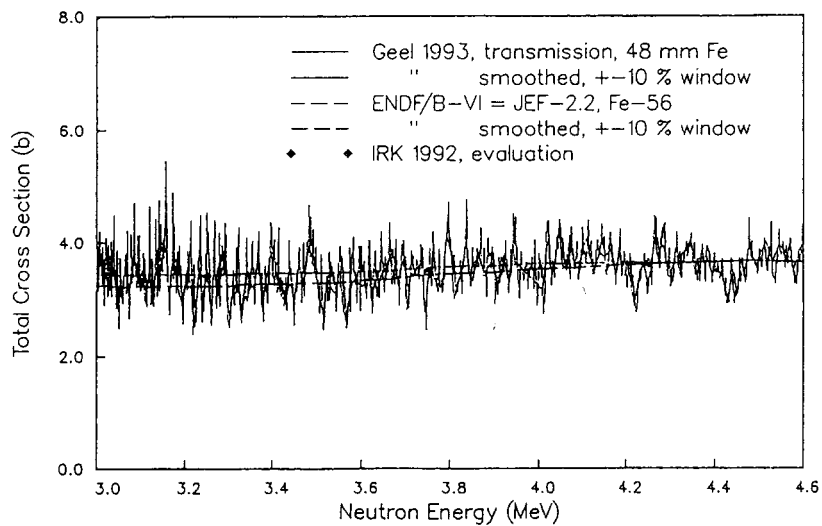


Figure 2

High-resolution total cross-section data for ^{56}Fe and smoothed energy-dependence (Geel and Oak Ridge measurements): genuine fluctuations are almost fully resolved below roughly 4 MeV. IRK evaluation is also shown.

Although less data with comparable resolution exist for the partial cross-sections of iron, we know from the resonance theory that the total cross-section resonance structure is present to quite some extent in all partial cross-sections, too. The structure of the elastic-scattering cross-section is practically the same up to the first inelastic threshold, i.e. for ^{56}Fe up to about 1 MeV, since all other channels (mainly capture) very little contribute in comparison. Other partial cross-sections, such as those for the (n,γ) , (n,n') , (n,p) , (n,α) reactions, mainly differ from the elastic-scattering cross-section in so far as both the potential part and the resonance-potential interference are lacking. Nevertheless the fluctuations are highly – and positively – correlated, resonance peaks appearing essentially at the same energies in all reaction channels. So it is not unreasonable to calculate self-shielding or other fluctuation effects for partial cross-sections with the fluctuations measured for the total cross-section, as long as their true fluctuations are not yet available. Then all partial cross-sections are taken as strictly proportional to each other, so that mere correlation is replaced by rigid proportionality. Benchmark calculations along these lines have been performed by L. Petrizzi (1994) and A. Hogenbirk (1995) with fluctuation factors extracted from the Geel data according to the recipe $f(E_i) = \sigma(E_i) / \bar{\sigma}(E_i)$, where $\bar{\sigma}$ is the smooth cross-section obtained by averaging the data within a suitable energy interval (“window”) centred at E_i (Fröhner 1994). The main result is that fluctuation effects are quite noticeable in the unresolved resonance region of iron up to about 4 MeV. In the sequel we describe theoretical studies that lead to the same conclusion and also allow a quantitative prediction of fluctuation effects for other structural materials.

2. Effect of cross-section fluctuations on transmission data

In order to see the relevance of cross-section fluctuations for shielding studies, let us consider the simplest kind of fluctuation effect, namely the enhancement of the energy-averaged transmission of a sample bombarded by a parallel beam of neutrons. The familiar exponential relationship $T = e^{-n\sigma}$ between transmission T , sample thickness (areal density of nuclei) n , and Doppler broadened total cross-section σ , is applicable only if the cross-section is so smooth, or the energy resolution so good, that the cross-section does not vary noticeably within the width of the resolution function (which in typical time-of-flight measurements is somewhat larger than the time channel width). In general the cross-section variation over the instrumental resolution function cannot be neglected. The simple exponential relationship between transmission and total cross-section must then be replaced by the cumulant expansion (see Appendix).

$$\begin{aligned}
\langle \exp(-n\sigma) \rangle &= \exp(-n\langle \sigma \rangle) \\
&\bullet \exp\left(+\frac{n^2}{2!} \langle (\sigma - \langle \sigma \rangle)^2 \rangle\right) \\
&\bullet \exp\left(-\frac{n^3}{3!} \langle (\sigma - \langle \sigma \rangle)^3 \rangle\right) \\
&\bullet \exp\left(+\frac{n^4}{4!} \left[\langle (\sigma - \langle \sigma \rangle)^4 \rangle - 3 \langle (\sigma - \langle \sigma \rangle)^2 \rangle^2 \right]\right) \quad (1)
\end{aligned}$$

This is the fraction of the beam passing the shield without collision. The angular brackets, $\langle \dots \rangle$, denote energy averages over the resolution function. The first exponential on the right side would be sufficient if the cross-section was constant and thus equal to the resolution-broadened cross-section, $\langle \sigma \rangle$, while the other exponential factors are corrections for the second, third, fourth, etc., moment (or rather cumulant) of the cross-section variation within the range of the resolution function. Their values depend on the sample thickness and on the relative size of the cross-section variation. Taking logarithms we get:

$$-\frac{1}{n} \ln \langle e^{-n\sigma} \rangle = \langle \sigma \rangle - \frac{n}{2} \langle (\sigma - \langle \sigma \rangle)^2 \rangle + \frac{n^2}{6} \langle (\sigma - \langle \sigma \rangle)^3 \rangle - + \dots \quad (2)$$

The left-hand side is what measurers of high-resolution data usually report as the experimental total cross-section. The right-hand side shows, however, that this is not equal to the true resolution-broadened cross-section, $\langle \sigma \rangle$, but that it is usually smaller, even for thin samples and good resolution. The difference is largest in the steeply rising and falling slopes of cross-section peaks, and smallest on top of the peaks and in the valleys between peaks.

In order to find the average cross-section behaviour the Geel data were smoothed by averaging the reported data within broad energy intervals of a 10% relative half width – “10% sliding window”. As shown in Figure 3, the smooth cross-sections thus obtained from the 16- and 48-mm data differed systematically by about 3% at 1 MeV and 1% at 3 MeV, apparently because of the resolution effect described by Equation 2. Denoting the smoothing by overbars, and the resolution broadening of the original high-resolution data by angular brackets as above, we obtain from Equation 2 in the second-order approximation

$$\overline{\sigma} = \overline{\langle \sigma \rangle} - \frac{n}{2} \left(\overline{\langle \sigma^2 \rangle} - \langle \sigma \rangle^2 \right) \quad (3)$$

where $\bar{\sigma}$ is the smoothed apparent cross-section and $\langle\bar{\sigma}\rangle$ the resonance-averaged true cross-section. We assume that the smoothing window is wide enough to contain a statistically representative sample of resonances. We can now insert, for a given neutron energy, both sample thicknesses n_1 and n_2 and both smoothed cross-sections $\bar{\sigma}_1$ and $\bar{\sigma}_2$ corresponding to the 16- and 48-mm data. The solution of the resulting two linear equations is:

$$\langle\bar{\sigma}\rangle = \frac{n_2\bar{\sigma}_1 - n_1\bar{\sigma}_2}{n_2 - n_1} \quad (4) \quad \langle\bar{\sigma}^2\rangle - \langle\bar{\sigma}\rangle^2 = 2\frac{\bar{\sigma}_1 - \bar{\sigma}_2}{n_2 - n_1} \quad (5)$$

Thus the corrected average total cross-section found is also shown in Figure 3 as a function of neutron energy. At about 1 MeV it is roughly 1% higher than the smooth cross-section computed from the 16-mm data.

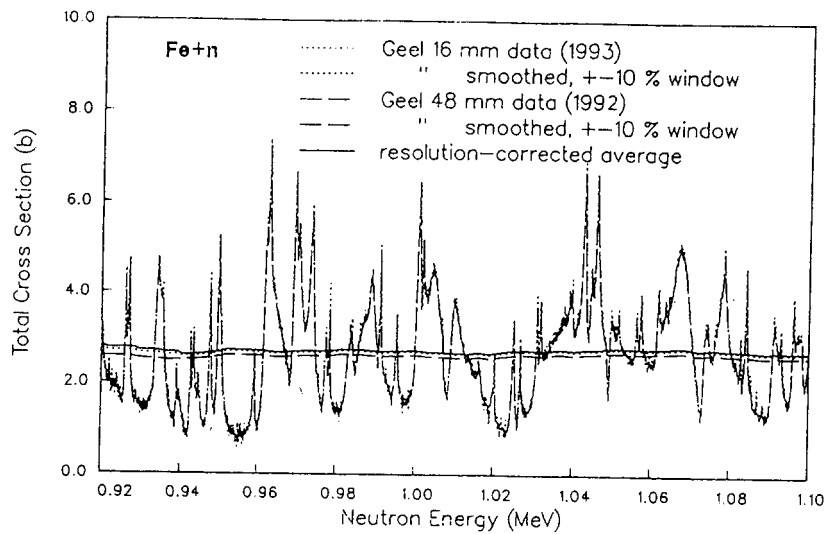


Figure 3
Total cross-section data measured at Geel showing systematic difference between smoothed 16- and 48-mm data.
The solid line is the average total cross-section after correction (cf. Equation 4).

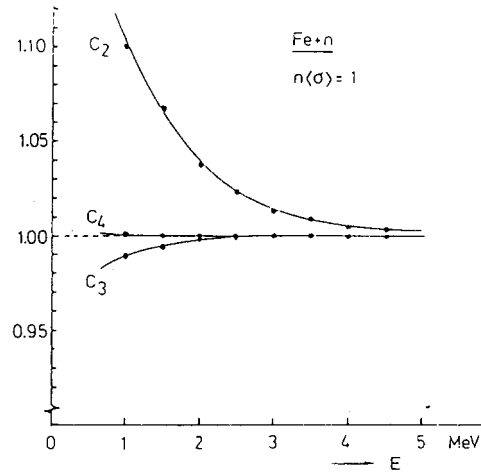


Figure 4

First three exponential correction factors in the average transmission expression (1), calculated for an effective sample thickness of one mean free path, $n(\sigma) = 1$, with cumulants obtained as sample averages in $\pm 10\%$ windows at various neutron energies between 1.0 and 4.5 MeV from the high-resolution 48-mm data measured at Geel.

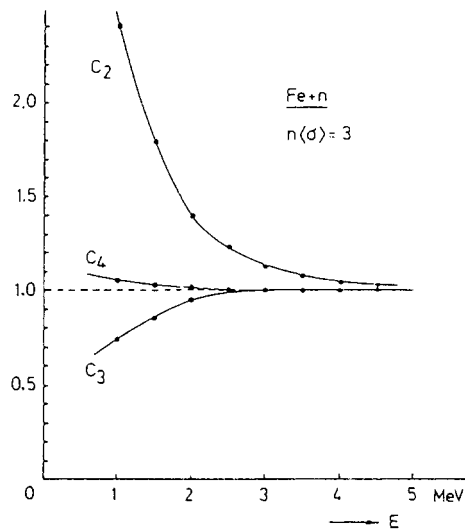


Figure 5

First three exponential correction factors in the average transmission expression (1), calculated for an effective sample thickness of three mean free paths, $n(\sigma) = 3$, with cumulants obtained as sample averages in $\pm 10\%$ windows at various neutron energies between 1.0 and 4.5 MeV from the high-resolution 48-mm data measured at Geel.

It can be seen from Figures 4 and 5 that the second-order approximation Equation 3 is adequate if the sample is not too thick. Both figures show the magnitudes of the 2nd, 3rd and 4th order exponential correction factors for iron samples with thicknesses of one and three mean free paths ($n\langle\sigma\rangle = 1$ and 3, i.e., a 37% and 5% transmission, the first value corresponding roughly to the 48-mm sample employed at Geel). The relative 2nd, 3rd and 4th moments were taken directly from the Geel 48-mm data as sample averages for a broad, rectangular resolution function of the 20% full width – “10 % sliding window”. According to Figure 3 this does not introduce any appreciable errors at 1 MeV where the cross-section structure is almost completely resolved; whereas at higher energies the sample moments – especially the higher ones – are smaller than the true moments. On the other hand all corrections become less important as one goes to higher energies. Above 4 or 5 MeV they are negligible for most practical purposes.

Obviously it is incorrect to calculate the transmission of a shield simply from resonance-averaged cross-sections (e.g., group cross-sections for infinite dilution) without fluctuation corrections. The moments of the cross-section distribution required for the corrections can be obtained from high-resolution transmission measurements such as those performed for iron at Geel. For other structural materials such high-resolution data are not available yet. The question arises whether cross-section fluctuations can be predicted from the nuclear reaction theory.

3. Theoretical prediction of mean-square fluctuations of the total cross-section

The general relationship between total cross-section and collision matrix (S-matrix) is:

$$\sigma = 2\pi\lambda^2 \sum_c g_c (1 - \text{Re}S_{cc}) \quad (6)$$

where $2\pi\lambda$ is the de Broglie wavelength of the relative motion of neutron and target nucleus, g_c the spin factor, and S_{cc} a diagonal element of the collision matrix (S-matrix). The sum is over all contributing (s-, p-, d-...wave) channels c . As the relationship is linear the resonance-averaged cross-section $\langle\sigma\rangle$ is given by the same expression with the S-matrix elements, S_{cc} , replaced by their averages over resonances, $\langle S_{cc} \rangle$, which can be obtained from an optical-model calculation.

An analytical expression for the variance of the total cross-section can be derived as follows. Because of $2\text{Re } S_{cc} = S_{cc} + S_{cc}^*$, we get from Equation 6:

$$\text{var } \sigma = \langle \sigma^2 \rangle - \langle \sigma \rangle^2 = (\pi\lambda^2)^2 \sum_c g_c^2 \left[\langle (S_{cc} + S_{cc}^*)^2 \rangle - \langle S_{cc} + S_{cc}^* \rangle^2 \right] \quad (7)$$

Causality demands that the S-matrix have no poles above the real axis in the complex energy plane. Poles corresponding to stable states (ground) lie on, and poles due to quasi-stationary states (resonances) lie below the real axis. This entails that $\langle S_{cc}^2 \rangle = \langle S_{cc} \rangle^2$, as easily proven for (broad) Lorentzian resolution functions by contour integration. The resulting expression for the variance can be written in the following form:

$$\text{var } \sigma = 2\pi\lambda^2 \sum_c g_c \left(\sigma_c^{CN} - \langle \sigma_c^{non} \rangle \right) \quad (8)$$

where
$$\sigma_c^{CN} = \pi\lambda^2 g_c \left(1 - \langle |S_{cc}|^2 \rangle \right) \quad (9)$$

is the optical-model compound nucleus formation cross-section and

$$\langle \sigma_c^{non} \rangle = \pi\lambda^2 g_c \left(1 - \langle |S_{cc}|^2 \rangle \right) \quad (10)$$

the resonance-averaged non-elastic cross-section which can be computed from average resonance parameters (strength functions or transmission coefficients) either with the many-level Breit-Wigner approximation which leads to width fluctuation corrections of the familiar Dresner factor type (cf. e.g., Moldauer 1980) or, more rigorously, with the GOE triple integral (Verbaarschot, Weidenmuller and Zirnbauer 1985).

For pure elastic scattering, $\sigma_c^{non} = 0$, the contribution of a given channel c to the variance of the total cross-section is simply proportional to the transmission coefficient $T_c \equiv 1 - \langle |S_{cc}|^2 \rangle$, which for weakly overlapping levels is twice the ratio of the average partial width to mean level spacing – an appealing and plausible result. Open non-elastic channels increase the level widths, hence the level overlap, which reduces the fluctuations. It should be noted that the contributions of the various reaction channels carry g_c^2 weights, whereas the contributions to the average cross-sections carry g_c weights. If a material contains several nuclides, with relative abundances a_j , the weights are respectively $a_j^2 g_c^2$ for

variances and $a_j g_c$ for cross-sections.

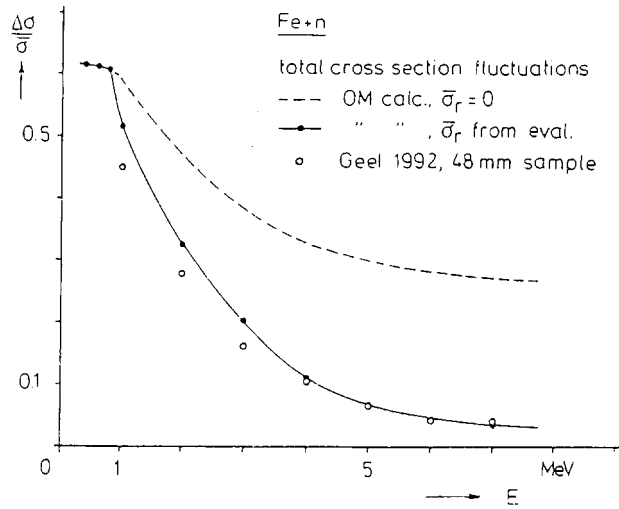


Figure 6

Calculated and observed relative standard deviations of the total cross-section of iron. The difference between the solid and dashed lines shows the impact of non-elastic – (n,n'), (n,p), (n,α) – reactions above the first inelastic threshold of ^{56}Fe at 0.86 MeV.

Figure 6 shows calculated and measured (relative) standard deviations for ^{56}Fe . The compound nucleus formation cross-sections were calculated with the spherical complex potential of Arthur and Young (1980) and the SCAT2 optical-model code (Bersillon 1981). The non-elastic cross-sections were taken from the evaluation of Vonach et al. (1992). Experimental standard deviations were directly obtained from the high-resolution Geel data (Weigmann et al., 1994) with a 10% sliding window as already described. Although the observed relative spread is about 10% smaller than the calculated one, the agreement is quite reasonable in view of the fact that first the calculation is exact only for pure compound reactions and for negligible Doppler and resolution broadening, and second that it was performed for ^{56}Fe while the empirical data are for natural iron with only 92% ^{56}Fe , – all of which tends to reduce the relative standard deviation $\Delta\sigma/\langle\sigma\rangle$. Above 4 MeV the relative spread is less than 10%.

It is concluded that the variance of the total cross-section in the unresolved resonance region can be calculated by standard optical-model and Hauser-Feshbach techniques from given average resonance parameters (strength functions and distant-level parameters, or the corresponding transmission coefficients and effective nuclear radii).

4. Theoretical prediction of partial cross-section fluctuations

Fluctuations of the partial cross-sections pose more complicated theoretical problems than those of the total cross-section. The fact that they are of comparable importance was shown by the shielding benchmark calculations at Frascati (Petrizzi 1994) and Petten (Hogenbirk 1995), in particular for the elastic and inelastic cross-sections. Figure 7 shows that the calculated neutron flux around 1 MeV in a 2-D ITER benchmark is about 15% lower if partial cross-section fluctuations are neglected, compared to when they are included (in the approximation of strict proportionality between total and partial cross-sections, with fluctuation factors taken directly from the high-resolution transmission data as explained before). The effect becomes insignificant above roughly 4 MeV.

The partial cross-sections for a nuclear reaction leading from an entrance channel c to an exit channel c' is not linearly related to the S-matrix as the total cross-section (see Equation 6) but by the bilinear relationship

$$\sigma_{cc'} = \pi\lambda^2 g_c |\delta_{cc'} - S_{cc'}|^2 \quad (11)$$

which is essentially the absolute square of probability amplitude for the transition $c \rightarrow c'$, the Kronecker symbol $\delta_{cc'}$ occurring because in-going and outgoing particles cannot be distinguished for elastic scattering without spin flip, $c=c'$. This expression can be averaged over resonances either with the Dresner integral approximation or, more rigorously, with the GOE triple integral, as mentioned already in connection with the non-elastic cross-section (see Equation 10).

The variance of the partial cross-section involves fourth-degree products of S-matrix elements which must be averaged over resonances. GOE averaging looks rather hopeless in view of the difficulties encountered already in the derivation of the triple integral for second-degree products. Nor does the Dresner integral approximation permit an easy generalisation to fourth-degree products.

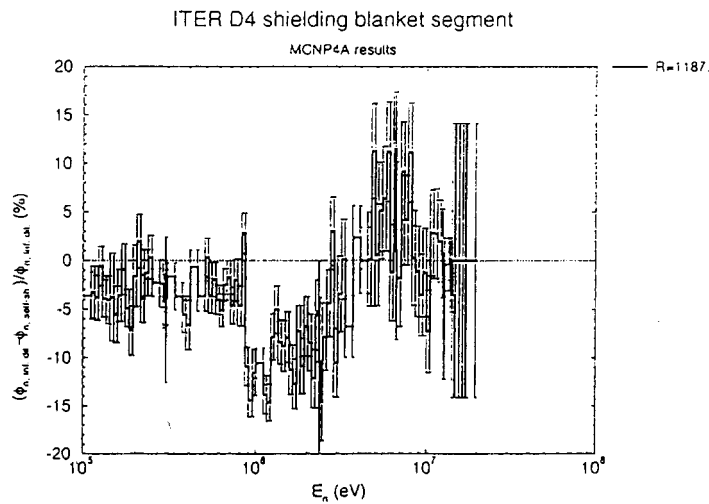
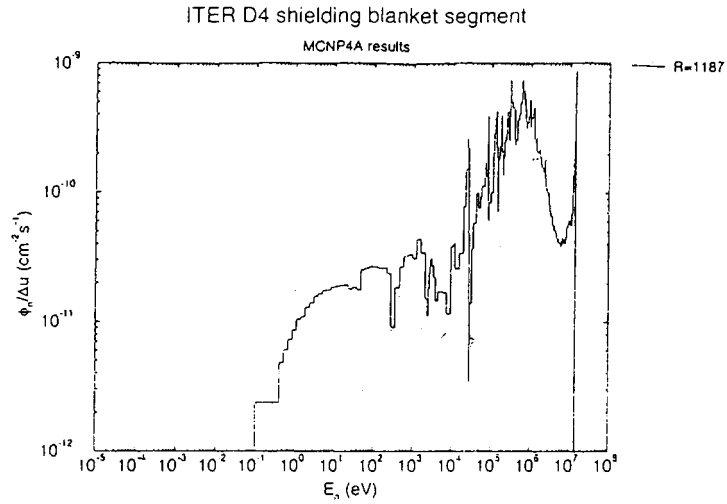


Figure 7
2-D ITER benchmark.
Neutron flux without self-shielding in the URR module of NJOY at R = 118.7 cm (upper figure). Relative difference between neutron flux with and without self-shielding in URR at R= 118.7 cm (lower figure). From A. Hogenbirk, EFF-DOC-351, December 1994.

More complicated cross-section functionals such as self-shielding factors involve even higher moments. An analytical treatment is possible at present only with drastic simplifications. One describes resonances of a given spin and parity in many-level Breit-Wigner approximation, with a smooth dilution cross-section added that represents other spins and parities of the same compound nucleus and also other admixed nuclides (Hwang 1965, Frölich 1965, cf. also Fröhner 1992).

An essentially rigorous computation of cross-section functionals in the unresolved resonance region is possible with Monte Carlo techniques based on the sampling of resonance ladders, i.e., of partial widths and level spacings from their level-statistical distributions (Porter-Thomas and Wigner or Dyson-Mehta), with subsequent calculations of Doppler broadened cross-sections. As an example Figure 8 shows a total cross-section distribution for Fe calculated with the Monte Carlo code SESH (Fröhner 1968) together with the experimental distribution of the Geel 48-mm data in a 10% window. Comparing calculation and measurement we must keep in mind that the Monte Carlo distribution is an expectation function, i.e., an average over many sampled ladders, whereas the observed distribution comes from the one ladder realised in nature. Partial cross-sections are readily sampled in the same manner. Doppler broadening is not a problem. All cross-section functionals of interest in the unresolved resonance region, averages, variances, covariances, higher moments, thick-sample transmission values, self-indication ratios, self-shielding factors, etc., can easily be computed from cross-section distributions (See also discussion and application to actinides by Fröhner 1991). It must be said, however, that the SESH code cannot be applied to cases with appreciable inelastic scattering – its extension to such cases, or the development of a more powerful code, is a task for the future.

5. Recommendations: information to be stored in evaluated files.

What has been said so far about predictability of structural-material cross-sections and their fluctuations, and about benchmarking utilising fluctuation factors extracted from high-resolution total cross-sections for elastic and inelastic scattering, leads to the following recommendations.

High-resolution total cross-section data should be stored unsmoothed and unthinned in the file. If they are available for the main isotopes of an element this is straightforward. If they are available only for the natural isotopic mixture they could be stored for all isotopes in the same way, which would ensure the correct outcome for the element and a reasonable representation at least for the main (even) isotopes. The energy range should extend from the end of the analysed

(“resolved”) resonance region up to 4 MeV. Above 4 MeV self-shielding effects are not very important and smoothed total cross-sections appear to be sufficient – *although with present storage capabilities we might as well file the unsmoothed cross-sections above 4 MeV too.* Above about 7 MeV, however, where the observed fluctuations are mostly due to counting statistics it seems better to store smoothed cross-sections so that users are not misled. This is all that is needed for the approximate (fluctuation factor) treatment of self-shielding effects outlined above.

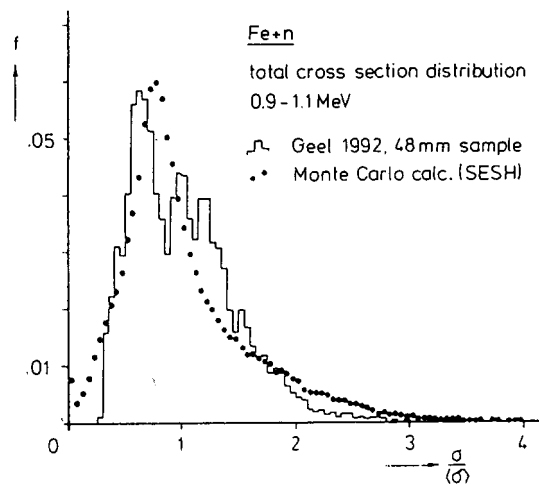


Figure 8

Histogram: total cross-section distribution sampled in a $\pm 10\%$ window centred at 1 MeV by the Geel 48-mm high-resolution measurement (cf. Figure 3). Solid points: total cross-section distribution obtained from Monte Carlo sampled resonance ladders.

More ambitious Monte Carlo methods based on resonance ladder sampling require transmission factors (strength functions) and effective nuclear radii for all relevant reaction channels and partial waves. As the number of contributing partial waves increases rapidly above the analysed resonance region (where $l = 0, 1, 2, 3$ are usually sufficient), as well as the number of open channels, and as existing ladder codes do not seem to be able to cope with more than four partial waves and more than one or two inelastic channels such computations appear to be still in the domain of basic nuclear physics rather than of nuclear technology. In principle the strength function information can be calculated from an appropriate optical model by the specialist but should not probably be stored in evaluated files at present. In any case this question might be considered by Subgroup 12 on *Nuclear Model Validation*.

6. Conclusions

This final report contains the main results from the work of NSC NEA/WPEC Subgroup 15. More details are given in the EFF progress reports, Subtask NDB1-6, of June 1993 and of November 1994, and in Fröhner's contribution to the Gatlinburg conference (1994). The following results have been obtained for medium-weight structural materials:

- A good data base of high-resolution total cross-sections in the non-analysed ("unresolved") resonance region has been established by the experimentalists at Oak Ridge and Geel, comprising iron, nickel, chromium, vanadium, titanium and molybdenum.
- A better theoretical understanding of cross-section fluctuations has been reached. It was realised that the variance of the total cross-section can be calculated from the Hauser-Feshbach theory. Furthermore, a cumulant expansion has been shown to link the average transmission and the moments of the total cross-section distribution. These results were used to investigate the energy dependence of cross-section fluctuations for iron. The result is that above 4 MeV the relative fluctuations are less than 10%.
- Benchmark calculations with and without fluctuations in the iron cross-sections have been performed both at Petten and at Frascati, with fluctuation factors extracted from high-resolution total cross-section data imposed also on partial cross-sections. The main result is that self-shielding effects are quite important up to 2 or 3 MeV but negligible above 4 to 5 MeV, confirming the theoretical assessment.

- The consequence for information storage in evaluated nuclear data files is that it is sufficient for most practical purposes to store the high-resolution data at least up to 4 MeV. Fluctuation factors can be extracted from these data and imposed on all interesting partial cross-sections for applications such as those made already in the NET and ITER context. New file formats or data types are not needed.

These results answer the questions which Subgroup 15 had to consider. It is therefore proposed to terminate the Subgroup.

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References

- E.D. Arthur and P.G. Young,
“Evaluated Neutron-Induced Cross-sections for $^{54,56}\text{Fe}$ to 40 MeV”,
Los Alamos Report LA-8626-MS (1980).
- O. Bersillon,
“The Computer Code SCAT2”, Report CEA-N-2227, Bruyères-le-Chatel
(1981).
- K. Berthold, C. Nazareth, G. Rohr, H. Weigmann,
“Very High Resolution Measurements of the Total Cross-section of Natural
Iron”, *Int. Conf. on Nucl. Data for Sci. and Technol., Gatlinburg 1994*,
La Grange Park (1994) vol. 1, p. 218.
- F.H. Fröhner,
“SESH – A FORTRAN-IV Code for Calculating Self-Shielding and Multiple
Scattering Effects for Neutron Cross-section Data Interpretation in the
Unresolved Resonance Region”, General Atomic Report GA-8380 (1968).
- F.H. Fröhner,
“Evaluation of the Unresolved Resonance Range of $^{238}\text{U}+n$ ”, *Nucl. Sci. Eng.*
111 (1991) 404.
- F.H. Fröhner,
“Theory of Neutron Resonance Cross-sections for Safety Applications”,
*Workshop on Computation and Analysis of Nuclear Data Relevant to Nuclear
Energy and Safety, ICTP Trieste 1992*, World Scientific, Singapore (1992);
separately available as report KfK 5073, Karlsruhe (1992).
- F.H. Fröhner,
“On Uncertainty Evaluation and Fluctuations in the Resolved and Unresolved
Resonance Regions”, *Int. Conf. on Nucl. Data for Sci. and Technol.,
Gatlinburg 1994*, vol. 2, p. 597.

- R. Frölich,
 “Theorie der Doppler-Koeffizienten ...”, Report KfK 367, Karlsruhe (1965).
- A. Hogenbirk,
 “Final Report of Shielding Calculations Performed at ECN Petten for ITER CTA Task D4/EU”, ECN-C-95-045 (1995).
- R.N. Hwang,
 “Doppler Effect Calculations with Interference Corrections”, *Nucl. Sci. Eng.* **21** (1965) 523; **52** (1973) 157.
- M.G. Kendall and A.S. Stuart,
The Advanced Theory of Statistics, Griffin, London (1969) vol. 1, ch. 3.
- A.M. Lane and R.G. Thomas,
 “R-Matrix Theory of Nuclear Reactions”, *Rev. Mod. Phys.* **30** (1958) 257.
- P.A. Moldauer,
 “Statistics and Average Cross-sections”, *Nucl. Phys.* **A344** (1980) 185.
- L. Petrizzi, private communication (1994).
- P. Ribon,
Ann. Nucl. En. **13** (1985) 209.
- J.M. Verbaarschot, H.A. Weidenmuller, M.R. Zirnbauer,
 “Grassmann Integration in Stochastic Quantum Mechanics: the Case of Compound-Nucleus Scattering”, *Phys. Reports* **129** (1985) 367.
- H. Vonach, S. Tagesen, M. Wagner and V. Pronyaev,
 “Evaluation of the Fast Neutron Cross-sections of Including Complete Covariance Information”, unpublished report, IRK Vienna (1992). cf. also
- V. Pronyaev, S. Tagesen, H. Vonach and S. Badikov,
 “Evaluations of the Fast Neutron Cross-sections of and Including Complete Covariance Information”, *Physics Data* **13-8** (1995).

Appendix

Cumulant Expansions

One way to specify a probability distribution $p(x)dx$ is to state its moments $\langle x \rangle, \langle x^2 \rangle, \langle x^3 \rangle, \dots$. The moments are the Taylor expansion coefficients of the moment generating function,

$$\langle \exp(kx) \rangle \equiv M(k) = \sum_{v=0}^{\infty} \frac{k^v}{v!} M^{(v)}(0) \quad (12)$$

Upon expansion of the exponential, in fact, $\langle x^v \rangle = M^{(v)}(0) \equiv (d/dk)^v M(k)|_{k=0}$. For many theoretical studies the moments are, however, less convenient than the cumulants. These are defined as the Taylor expansion coefficients of the logarithm of the moment generating function,

$$K(k) \equiv \ln M(k) = \sum_{v=0}^{\infty} \frac{k^v}{v!} M^{(v)}(0) \quad (13)$$

The v -th cumulant is $K^{(v)}(0) = (d/dk)^v \ln M(k)|_{k=0}$. After some straightforward algebra we find

$$\begin{aligned} K^{(0)}(0) &= 0, \\ K^{(1)}(0) &= \langle x \rangle, \\ K^{(2)}(0) &= \langle (x - \langle x \rangle)^2 \rangle, \\ K^{(3)}(0) &= \langle (x - \langle x \rangle)^3 \rangle, \\ K^{(4)}(0) &= \langle (x - \langle x \rangle)^4 \rangle - 3 \langle (x - \langle x \rangle)^2 \rangle^2, \dots \end{aligned} \quad (14)$$

Inserting these cumulants into Equation 13, exponentiating and putting $k = -n$, $x = \sigma$, we obtain the expression for the average transmission, in Equation 1. If the cross-section is a sum of independently fluctuating contributions (from various resonance sequences and nuclides), $\sigma = \sum_j \sigma_j$, the average transmission factorises into a product of individual average transmissions for the various σ_j , with appropriate areal densities $n_j = a_j n$, $n = \sum_j n_j$:

$$\langle \exp(-n\sigma) \rangle = \prod_j \langle \exp(-n_j \sigma_j) \rangle$$

Each factor of the product can be expressed in turn by a cumulant product expansion of the type displayed in Equation 1. This makes application to superpositions of resonance sequences and to isotopic mixtures quite easy. The generalisation to correlated variates, existence conditions and other questions concerning cumulants are discussed e.g., by Kendall and Stuart (1969).