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NSC Subgroup 15 – Self-Shielding in the Unresolved Region
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CROSS SECTION FLUCTUATIONS AND SELF-SHIELDING EFFECTS IN THE UNRESOLVED RESONANCE REGION

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ABSTRACT. NEANSC Subgroup 15 has 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

- the new data base consisting of high-resolution transmission data for iron, nickel and vanadium measured at Oak Ridge and Geel;
- the improved theoretical understanding of cross section fluctuations, including their prediction, that has been derived from 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 Hauser-Feshbach theory show that self-shielding effects are important up to 4 or 5 MeV of 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 average resonance parameters are available. Needs for further work on techniques and codes were identified but the main tasks of the subgroup appear to be fulfilled.

1. The High-Resolution Transmission Data

High-resolution transmission measurements performed on iron, nickel and, most recently, on vanadium at Oak Ridge and Geel reveal strong resonance structure of the total cross section extending far into the so-called unresolved resonance region. For iron the boundary between the so-called resolved (i. e. fully analysed) resonance region and the unresolved (better: unanalysed) resonance region is at about 0.86 MeV which is the first inelastic threshold of ^{56}Fe. The resonance structure diminishes gradually above that energy but only above 4 MeV are the relative fluctuations smaller than 10 %. As the resonance structures and ranges of analysed and unanalysed resonances are similar for all medium-weight structural materials, the results obtained for iron are applicable also to nickel, chromium, and vanadium. Nonnegligible self-shielding effects are therefore expected up to about 3 to 5 MeV for all these elements.

A first question was: Is the observed cross section structure really the true resonance structure or is it affected by intrumental resolution and counting statistics? In the Geel data it was easy to verify that above about 7 MeV most of the observed fluctuations were simply due to counting statistics (Fig. 1). From 7 MeV down to 4 MeV true fluctuations are seen but smoothed to some extent by limited instrumental resolution. (Fig. 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 (Fig. 3).

2. Improved Theoretical Understanding of Cross Section Fluctuations

The conclusion that above about 4 MeV the fluctuations of the total cross section are unimportant for most practical purposes, and that below 4 MeV most of the true structure was resolved in the high-resolution data was corroborated by theoretical calculations. Hauser-Feshbach theory permits estimation of the mean and the variance of the total cross section as a function of neutron energy from average resonance parameters and effective nuclear radii for the various partial waves. The relevant expressions are

$$\langle \sigma \rangle = 2\pi \bar{\lambda}^2 \sum_c g_c (1 - \mathrm{Re}\,\langle S_{cc} \rangle), \tag{1}$$

for the mean and

$$\mathrm{var}\,\sigma = 2\pi \bar{\lambda}^2 \sum_c g_c (\sigma_c^{CN} - \langle \sigma_c^{non} \rangle), \tag{2}$$

for the variance, where $2\pi\bar{\lambda}$ is the de Broglie wavelength of the relative motion of neutron and target nucleus, g_c the spin factor, $\langle S_{cc} \rangle$ a diagonal element of the optical-model (or resonance-averaged) S matrix, and the sums are over all contributing (s-, p-, d-...wave) channels c. The compound nucleus formation cross section, $\sigma_c^{CN} = \pi\bar{\lambda}^2 g_c (1 - |\langle S_{cc} \rangle|^2)$, and the resonance-averaged nonelastic cross section, $\langle \sigma_c^{non} \rangle = \pi\bar{\lambda}^2 g_c (1 - \langle |S_{cc}|^2 \rangle)$, are to be calculated as usual, the former from an optical model, the latter from optical-model transmission coefficients (equivalent to strength functions) either rigorously with the GOE triple integral[3] or with the familiar Dresner integral approximation for the width fluctuation correction. Open inelastic channels increase the level widths, hence the level overlap, and thus reduce the fluctuations at higher energies. Fig. 4 shows calculated and measured relative standard deviations for ^{56}Fe. The measured points are only about 10 % below the calculated curve which indicates that Doppler and resolution broadening are not very important, hence most of the true structure is resolved. Above 4 MeV the relative fluctuations are below the 10 % level and thus unimportant for most practical purposes.

3. Benchmark Calculations

Benchmark calculations involving fluctuating iron cross sections were performed by A. Hogenbirk (Petten) and L. Petrizzi (Frascati). These authors used fluctuation factors that had been extracted from the high-resolution iron transmission data measured at Geel as follows. The fluctuating total cross sections derived from the transmission data can be written as a product of an energy average and a fluctuating factor,

$$\sigma(E) = \bar{\sigma}(E) f(E). \tag{3}$$

The smooth cross section was determined by averaging the experimental cross sections in a ±10 % energy interval around the energy E of the data point. The factor $f(E)$ is then simply the ratio of observed and smoothed cross section. The factors $f(E)$ thus obtained were then used to impose the same fluctuations as observed for the total cross section also on all relevant partial cross sections. The actual positive correlation between total and partial cross section structure was thus replaced by strict proportionality. Although this is not quite correct – resonance peaks in different reaction channels, although appearing at the same energies with the same widths, have essentially uncorrelated heights – it is expected to be an adequate approximation of partial cross section fluctuations in transport calculations or activation studies.

The main result of these benchmark calculations was that there are nonnegligible effects up to roughly 3 MeV, which is consistent with the predictions based on the high-resolution data and on Hauser-Feshbach theory (see Fig. 5).

4. Information to be Stored in Evaluated Files

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 be 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 one might as well file the unsmoothed cross sections also above 4 MeV. Above 7 MeV or so, however, where the observed fluctuations are mostly due to counting statistics it seems better to store smoothed cross sections so that users are not mislead. This is all that one needs for the approximate (fluctuation factor) treatment of self-shielding effects outlined above.

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 $\ell = 0,1,2,3$ are usually sufficient), and also 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. The strength function information can in principle be calculated from an appropriate optical model by the specialist but should probably not be stored in evaluated files at present. In any case this question might be considered in Subgroup 12 on Nuclear Model Validation.

5. Conclusions

This status report is quite brief. For more details see the EFF progress reports, Subtask NDB1-6, of June 1993 and of November 1993, F. Fröhner's contribution to the Conference on Nuclear Data for Science and Technology, Gatlinburg, May 1994, and the NSC Subgroup 15 report of November 1994. The following results have been obtained for medium-weight structural materials:

- A good data base of high-resolution total cross sections in the nonanalysed ("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 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 suffices 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.

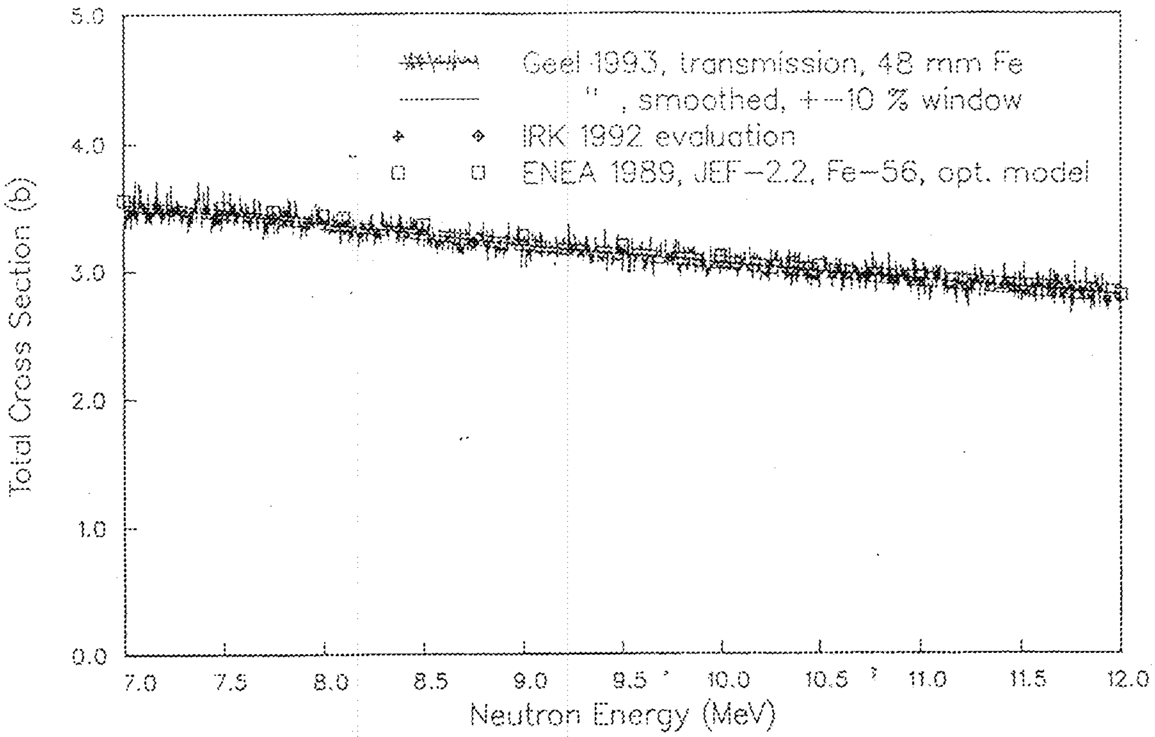

Fig. 1. High-resolution total cross section data for ^{56}Fe and smoothed energy dependence with confidence band indicating standard uncertainty from counting statistics (Geel measurements): genuine fluctuations are drowned in noise from counting statistics above 7 MeV. IRK and JEF evaluations are also shown.

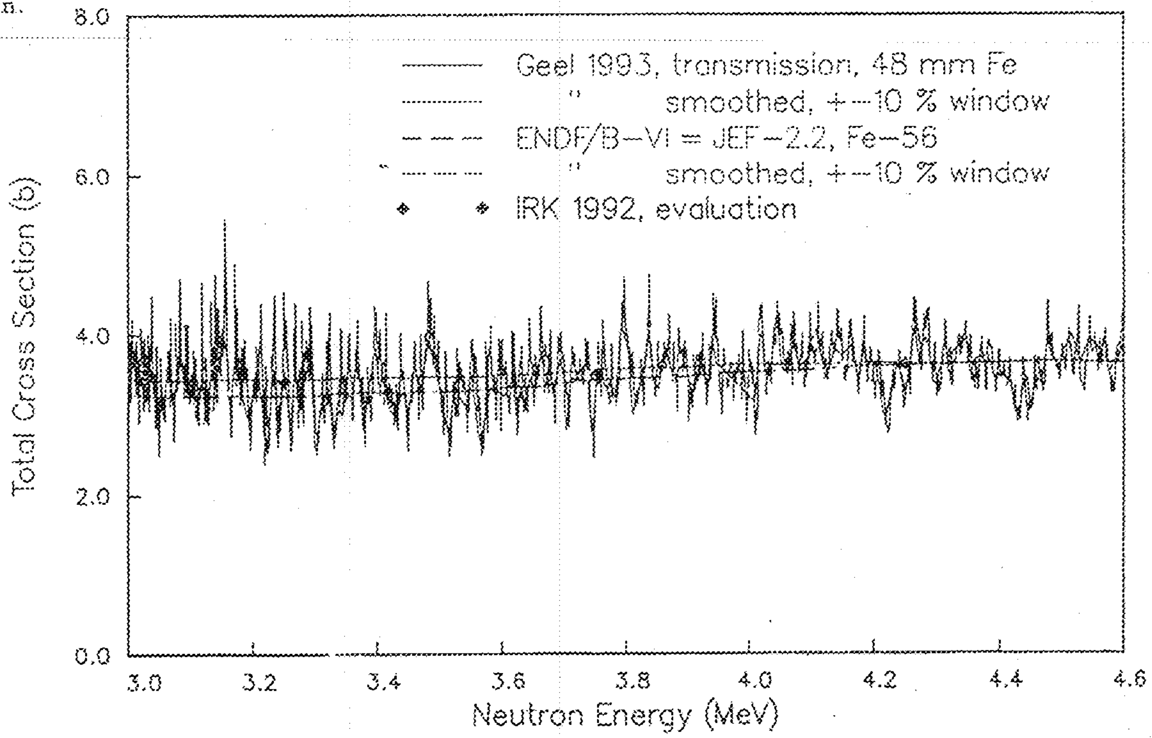

Fig. 2. High-resolution total cross section data for ^{56}Fe and smoothed energy dependence (Geel and Oak Ridge measurements): genuine fluctuations are almost fully resolved below roughly 4 MeV. The IRK evaluation is also shown.

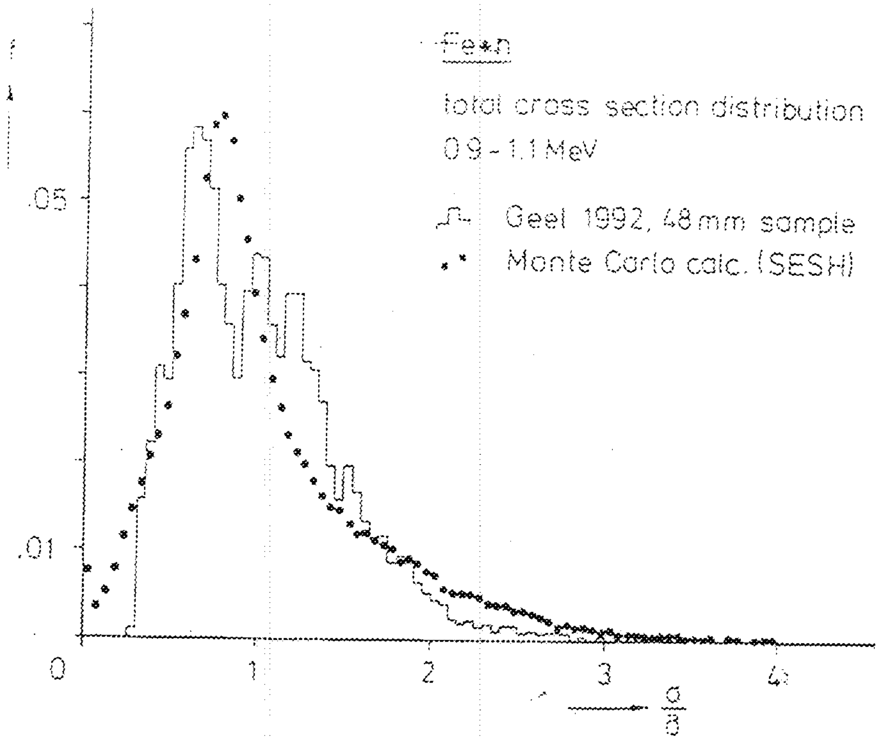

Fig. 3. Observed distribution of total cross section in a ±10 % window around 1 MeV (iron high-resolution data from Geel) and Monte Carlo calculation based on resonance ladder sampling relying on strength functions and effective nuclear radii from the resolved resonance region.

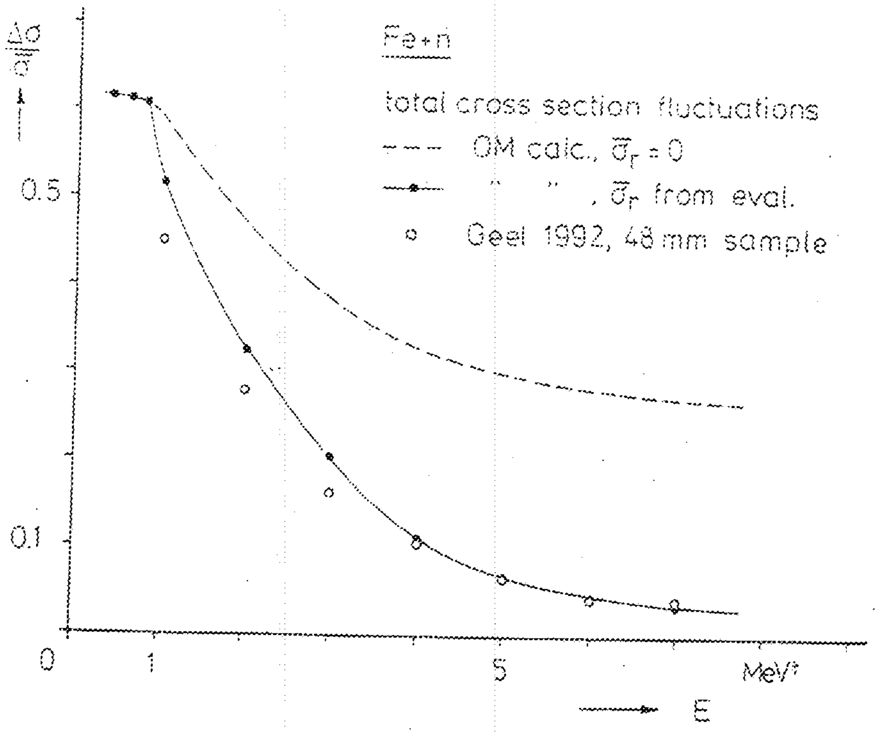

Fig. 4. Calculated and observed relative standard deviations of the total cross section of iron. The difference between the solid and dashed lines shows the impact of nonelastic – (n,n'), (n,p), (n,α) – reactions above 0.86 MeV (first inelastic threshold of ^{56}Fe).

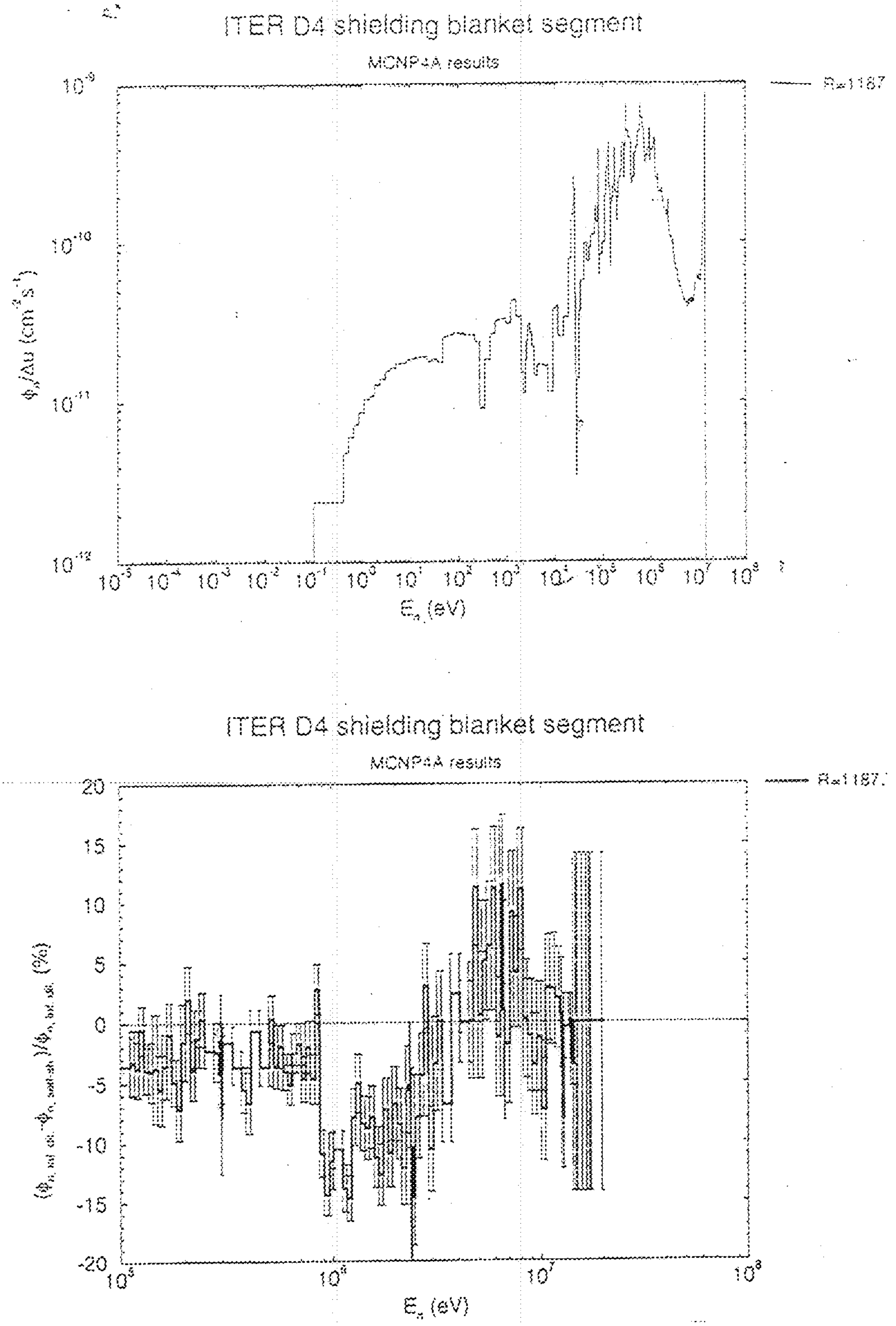

Fig. 5. 2D ITER benchmark. Neutron flux without self-shielding in the URR module of NJOY at $R =$ 118.7 cm (upper figure). Relative difference between neutron flux with and without self-shielding in URR at $R=$ 118.7 cm (lower figure). From A. Hogenbirk, EFF-DOC-351, December 1994.