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EXPERIENCE WITH NEUTRON SPECTRUM UNFOLDING CODES

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SUMMARY

This report reviews the experience obtained in the past few years with the following unfolding codes:

SAND-II, CRYSTAL BALL, RFSP-JUL, and STAY'SL.

The main emphasis is on the comparison of these codes, based on practical experience with application of these codes under comparable conditions.

KEYWORDS

NEUTRON SPECTRA

SPECTRA UNFOLDING

ACTIVATION DETECTORS

C CODES

R CODES

S CODES

GROUP CONSTANTS

EXPERIMENTAL DATA

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1. INTRODUCTION

Experimental information on a neutron spectrum can be obtained from a set of experimental reaction rates, obtained with activation and/or fission detectors.

The advantage of this type of detectors is that in general their dimensions can be small with respect to proportional counter tubes which sometimes are also used for neutron spectrum determination.

Also the insensitivity of activation detectors to gamma ray radiation, and the wireless operation are advantages.

The irradiation times which are needed for a particular set of activation detectors depend on the neutron flux density and the mass, type and nuclear data of the detector material.

The detectors are selected in such a way that a suitable product radio-nuclide is obtained.

After the irradiation the activity of each detector of the set is measured, from which the activity per atom at saturation in the considered neutron field is derived.

The choice of activation detectors in a set is also influenced by the type of neutron field. A thermal neutron flux density spectrum requires other detectors than e.g. a fission spectrum. The suitability of a particular reaction for a certain spectrum depends mainly on its cross section as a function of energy. Relatively large cross section values should be present at those energies where neutron spectrum information is required. Furthermore the cross section shapes of the reactions should all be different and well known.

The latter remark restricts in practice the size of the detector set to a rather simple one, especially if it is considered that each reaction contributes to the reliability of the resulting neutron spectrum. Practical problems like unsuitable half-lives and difficulties with counting give a further restriction to the composition of the set, so that for general purpose reactor metrology activation sets of 20 or less reactions can be used.

In the case that the activities at saturation of an activation detector set are available, an unfolding procedure has to be performed to obtain the neutron flux density as a function of the energy from the experimental reaction rates at saturation.

Due to the rather small number of activation reactions in an activation

set, the number of flux density groups which can directly be derived is also small. Therefore another approach was required to have a better representation of the neutron spectrum in some more groups. This was found by insertion of additional information on the input of the program, which is required for the calculation of the output spectrum (or solution spectrum). The additional information consists of the best estimate of the neutron spectrum in which the activation detector set was irradiated.

The computer programs which are applied for the calculation of the output spectrum are often called unfolding programs. These programs perform the spectrum calculations generally with a rather fine group structure of the energy scale, so that the number of energy groups is much larger than the number of detectors.

The calculation procedure results in an output spectrum which is a modification of the input spectrum.

Various procedures for modifications are applied in the unfolding programs, but a property of all the programs is that the reaction rates of the detector set (experimental values) are compared with calculated reaction rates, obtained for the neutron spectrum of interest and an available cross section library.

If appreciable differences are found in the comparison of experimental and calculated reaction rates, the unfolding algorithm of the program will modify the input spectrum data in such a way that in general this difference becomes smaller.

The modification procedure implies in some cases internal rules, which determine some properties of the output neutron spectrum.

In some unfolding programs the modification of the input spectrum is performed in a number of iterations, while in other programs in principle only one step is required to achieve the output spectrum.

The role of the various reactions which are applied in the calculation of the solution spectrum can be influenced by the use of statistical weights.

The decision whether "a" solution or "the" solution has been achieved is not a unique procedure.

In the older programs rather crude criteria were applied, while more recent programs give the solution on the base of a least squares calculation in which all uncertainty contributions are considered.

The uncertainty information can comprise variance and covariance contri-

butions for the three input data groups (reaction rates, input spectrum, and cross section values).

The output data of the programs, which apply extensive uncertainty information in the input, can supply also uncertainty data for the output spectrum.

An estimate of the uncertainty of a solution spectrum obtained with an unfolding code in which only the uncertainty of some data was applied in the input can be obtained with a Monte Carlo procedure. In this procedure the influence on the solution of the uncertainty introduced for certain input parameters can be calculated.

An other procedure demonstrates the improvement ratio for a certain input set for an unfolding code.

The results of an unfolding procedure will be influenced by three contributions. These are:

- the input data;
- the mathematical properties of the unfolding procedure;
- the guidance (quality decision) by the unfolding physicist.

In the following part of the report the influence of the three contributions will be discussed. It may be clear that the influences of the three contributions cannot always be separated.

2. INPUT DATA

2.1. Problem independent input data

All the unfolding procedures under consideration require (evaluated) cross section data for the applied reactions in an unfolding run.

The cross section data are in most cases available in the form of a library.

Some unfolding programs need the cross section data as point values, while other programs apply group cross section values in the calculations. The libraries which were available during the execution of our work were several: SAND-II libraries, the ENDF/B-IV dosimetry file [1], and the DOSCROS77 library [2].

All these cross section libraries are available in a (SAND-II) group structure which comprises 620 groups with 45 groups per decade of energy below 1 MeV, and groups with a width of 100 keV between 1 and 18 MeV [3].

The data on the ENDF/B-IV dosimetry file in the SAND-II structure originate from the ENDF/B-IV dosimetry file TAPE412, which is available as point cross section values with prescribed interpolation rules for the smooth part and with resonance parameters for the resonance regions.

The 620 group structure is fine enough to be rather independent of the weighting spectrum, which is applied to calculate the group cross section.

In the case that the cross section data have to be corrected for the effect of neutron selfshielding, the 620 group structure is in principle too coarse [4], but in most cases reasonable results will be obtained.

Some unfolding programs perform the calculation with a much coarser group structure (i.e. 50 or 100 groups). The use of these programs for general purpose reactor metrology spectrum unfolding makes it necessary to calculate group cross sections in the appropriate structure.

The weighting spectrum which is required in these calculations should be accurate, otherwise important errors may be introduced in the calculations. This holds especially for spectrum regions with large local flux density changes.

If the spectrum resulting from the unfolding deviates clearly from the weighting spectrum, extra calculations of adapted group cross section may be required.

The requirements of the input (weighting) spectra are discussed in 2.2.2.

In some unfolding programs uncertainty data of the cross section data can be inserted.

In one of the unfolding codes (STAY'SL) detailed variance and covariance data can be applied and another code (SANDPET) uses rather simple uncertainty data. Detailed cross section uncertainty data were not yet available. A rather simple library with uncertainty data has been presented some years ago by McElroy [5]. In this library a rough group structure is applied: 15 groups from 10^{-12} to 18 MeV. In each group the error is assumed to be constant and independent of the values presented for other groups.

Data are available in this library for a series of metrology reactions. In our study this library has been used without updating for changed and improved cross section data, which became available more recently. In some unfolding codes corrections can be made for the presence of covers surrounding the activation or fission detectors during the irradiation. For these correction calculations some special cross section sets are required, which were written also in the cross section libraries.

2.2. Problem dependent input data

2.2.1. Reactions and activity data

In all unfolding codes a series of reaction rates for different materials have to be given in the input. The reaction rates are specified in terms of activities at saturation per target atom. These values are obtained from counting results with aid of a series of calculations with various constants and conversion factors. In several unfolding programs also the uncertainty of the activity values can be inserted.

The estimate of the uncertainty of the input activity data is rather complex. The reproducibility of activity determinations can in general be determined rather well, but the influence of systematic effects on the uncertainty is often questionable due to lack of knowledge on the contribution of various sources (i.e. perturbation of irradiation field, uncertainties related to counting systems, uncertainties in nuclear data, etc.).

In two unfolding programs (SAND-II and CRYSTAL BALL) corrections can be made for the absorption of incident neutrons in covers which surround the target material of interest during the irradiation. The correction is based on a simple exponential attenuation.

2.2.2. The input spectrum

All four unfolding codes require an input spectrum. This input spectrum should contain all information which is available for the experiment position under consideration. The information which is available for a neutron spectrum at a position of interest can originate from various sources.

- The results of detailed reactor physics calculations are probably the best.
- In some cases good results can be obtained with theoretical functions (e.g. for a well moderated neutron spectrum the Maxwell function coupled to a $1/E$ distribution).
- The comparability of the position of interest with a position with known neutron input spectrum can lead to select these data as input spectrum.
- The experience or intuition of the unfolding physicist is used when other information seems insufficient or unreliable.

The spectrum information which is obtained from physics calculations is often supplied for an energy interval which is smaller than the energy interval which is required for the unfolding.

In the detector set for unfolding often detectors are applied for thermal neutrons as well as detectors which detect fast neutrons above 10 MeV. For this reason the calculated spectrum has to be extrapolated.

For the extrapolation of a calculated reactor neutron spectrum a representation of the fission spectrum can be applied in the fast neutron region. At the low energy side various extrapolation functions can be used. For a well moderated thermal reactor a $1/E$ distribution coupled to a Maxwellian is often applied.

In this extrapolation the joining energy of both distributions and the temperature of the Maxwellian are important parameters to obtain the correct ratio of thermal and intermediate neutron contributions.

For the extrapolation on low energy sides of fast reactor spectra no general relation is available and background information is required to find an acceptable spectrum shape.

The values which are obtained from the physics codes for spectrum calculations are often group flux density values for rather broad energy groups. Extrapolation of these data is not a straightforward matter. Also the calculations of the group cross sections in energy regions with narrow

peaks in the cross section curve and the actual spectrum are rather unreliable. For this reason it can be tried to obtain a more smooth spectrum. This spectrum has to be made in such a way that the group flux density values of the smoothed spectrum and the original calculated spectrum are the same.

For such a spectrum it can be assumed that the original information is still present in acceptable form and that the disappearance of the steps in the flux density makes the spectrum more probable from a physics point of view.

A smooth spectrum can be obtained by conversion of the group flux density values in point flux density values.

For this conversion several methods can be applied, but a reasonable choice seems to be for the groups with a width of $\Delta E = E_U - E_L$ and a value ϕ_g for the group flux density $E = \Delta E / \Delta u$ and the corresponding flux density value $\phi_E = \phi_g / \Delta E$. The value Δu is given by

$$\ln E_L - \ln E_U.$$

A smooth spectrum can be obtained by linear interpolation of the point flux density values and also the extrapolation can easily be performed. For the interpolation a straight line function through the logarithms of the energy and flux density values can be used.

Condensation of the smooth data into the original structure will show differences.

Small changes in the point flux density will effect the results of the condensation; in this way with trial and error a smooth spectrum with correct group values can be obtained.

The smooth spectrum data can now also be converted to a coarser group structure for the unfolding programs with a rather small number of groups.

2.2.3. The convergence criterion

The various unfolding codes apply different criteria to decide whether further calculations in a next iteration step are required.

In one program (STAY'SL) the solution spectrum is calculated on basis of a direct least squares procedure in one single step. Here the uncertainty data of all input data are applied in the calculation.

The other unfolding programs (SANDPET, RFSP-JUL, CRYSTAL BALL) have the possibility to insert only the uncertainty data of the input activity or they require no uncertainty data at all (original SAND-II version).

The ratio of the input and the calculated activity can be computed and the standard deviation of the ratios of an input set can be calculated for the spectrum of interest (input, intermediate or output).

If the calculated spectrum is a good approximation to the actual spectrum of irradiation position, the standard deviation will be small.

Due to counting statistics and the conversion data applied in the activity determinations an activity value with some uncertainty will be obtained. This can be the reason that even for the case that the true spectrum and the calculated spectrum are the same, a relatively high standard deviation will be found (an uncertainty value for the activity of 2% is estimated here).

In the calculation of the activities in the unfolding procedures a cross section library is used. These cross section data are not completely exact and will show also uncertainties. These cross section uncertainties should also be considered in the interpretation of the standard deviation of A_m/A_c .

A measure which seems to be better suited for observing the fit between the input reaction rates and calculated reaction rates is the difference between these two values divided by its standard deviation. The standard deviation should comprise the contributions of the input and the calculated reaction rate uncertainties [6]. A value much larger than 2 for this measure shows that a significant difference for the two reaction rate values is found for the spectrum of interest.

The overall performance of the detector set in the spectrum of interest can be obtained as the square root of the sum of the squares of the differences divided by their standard deviations, divided by the number of detectors (the so called "average relative deviation").

This value should be near 1, if no differences exist between the true and the calculated spectrum. This means that the average difference will be of the order of the standard deviations of the series.

In the case that the latter value is near 1, it means not directly that an acceptable solution has been obtained, because too much structure or other physically unrealistic patterns might have been generated by the unfolding procedure. For this reason the shape of the solution spectra should always be considered in combination with the convergence criterion. The acceptability of the spectrum should always finally be judged from a physics point of view.

3. THE UNFOLDING CODES

The following unfolding programs have been applied:

- CRYSTAL BALL |7|
- RFSP-JÜL |8|
- SANDPET, a modification of SAND-II |9|
- STAY'SL |10|.

These four programs apply each a different algorithm to calculate the solution spectra. The algorithms are not discussed here, but described in the program manuals; three programs are reviewed in |11|. They are all suited to calculate a complete reactor spectrum.

There are important differences and limitations to all the programs which will be discussed in the following part.

The presentation of the results and the plotting of the neutron spectrum data was performed with a few small utility programs.

The calculations with the unfolding programs were performed with a CDC CYBER-175 computer.

3.1. CRYSTAL BALL |7|

The program CRYSTAL BALL needs a cross section library which has an identical format as the library which is used in the SAND-II program. The cross section library can be written by the utility program of CRYSTAL BALL named XSTAPE.

A difference between the SAND-II and CRYSTAL BALL libraries is that the SAND-II library contains group cross section data, and the CRYSTAL BALL library point cross section data. For this reason we modified the program CRYSTAL BALL in such a way that the SAND-II library could be applied directly.

The input data have to be given in a prescribed format. It is possible to perform automatically corrections for the presence of detector covers (Au, B or Cd).

The values of the parameters required in the input for the speed of convergence are very often not well chosen, so that trial runs are needed to obtain the desired performance.

In the program performance one single and reliable reaction has to be specified in the input. This reaction has to be indicated with the so called detector importance index. In our calculations we used a reaction with low uncertainty data.

The input spectrum in the series of calculations was always supplied in the 620 groups format of SAND-II. The several other input possibilities for the input spectrum information were not supplied.

The convergence criterion which is applied in CRYSTAL BALL and printed as average relative deviation seems to be a good criterion. It is defined as

$$\text{ARD} = \left\{ \frac{1}{n} \sum_{i=1}^n \left(\frac{A_i^m - A_i^c}{s_i^m} \right)^2 \right\}^{\frac{1}{2}}$$

where

- n = number of input reaction rates;
- A_i^m = input reaction rate;
- A_i^c = calculated reaction rate for spectrum of interest;
- s_i^m = estimated uncertainty in $A_i^m - A_i^c$.

A drawback of this convergence parameter can be present if the set of $(A^m - A^c)/s_i^m$ values comprises one large value. In this case a too low value for this ratio is obtained for all other reactions, since the solution is determined by the ARD, which is the root mean square value of all these ratios.

A small disadvantage of the present version of the program is that the ratio of input reaction rate and calculated reaction rate for the input spectrum is not printed.

The input spectrum data can be applied in several formats and forms. Extrapolation of these data on the low energy scale and high energy scale can be performed and also the interpolation between energy points is taken care of in the program. In these calculations an output of SAND-II (without spectrum modification) was applied as input spectrum for CRYSTAL BALL.

The execution of the program requires a computer with rather large capacity (~64 k memory positions). The actual calculations require much more computer time than the other programs. This is very pronounced if a series of iterations has to be performed. The number of iterations can be adjusted with some special input parameters. A good value for these parameters can save computer time when more calculations for a particular input deck have to be performed. A typical calculation time for the calculations considered here is 60 s.

3.2. RFSP-JÜL |8|

The program RFSP-JÜL needs a cross section library consisting of energy values with accompanying cross section values.

The program performs the interpolations which can be done in two ways. In our study the cross section library in the SAND-II format was modified, so that these data could be used as input for RFSP-JÜL.

The input cards have to be supplied in a prescribed format.

The speed of convergence can be adjusted with a special input parameter called ω . The actual value of ω is problem dependent and has to be chosen with care from trial runs, to obtain the output in a reasonable number of iterations.

The program cannot correct automatically for covers which are applied around the detectors during irradiations. In these calculations this was solved by applying these corrections directly to the input cross section data.

The input spectrum has to be supplied in a rather coarse energy structure which is not extrapolated in the program. In these calculations we used 75 groups or less.

The point flux density can be interpolated with four different methods which have to be specified in the input |8|.

The actual spectrum input data in some of our final calculations were obtained with a utility program of STAY'SL where the same group structure is applied.

The convergence criterion of RFSP-JÜL is not so convenient if input uncertainties are applied. For this reason the output data were interpreted in terms of the parameter ARD as applied in CRYSTAL BALL.

The execution of the program needs a computer with large capacity (≈ 66 k memory positions). In this respect it is the largest program of the four programs considered here.

The computer time needed for a typical run for this report is about 4 s. The number of iterations does not effect this time appreciably.

3.3. SAND-II |9|

In the calculations presented here a somewhat extended program version of SAND-II was applied. This extended version is named SANDPET. The extensions comprise the error calculations with a Monte Carlo procedure,

the application of input uncertainties for the reaction rates and the calculation of the improvement ratio.

The principle of the Monte Carlo procedure and the input uncertainty application is the same as described in [12], [13], and [14]; the realization method is somewhat different.

The principle of the improvement ratio calculations is described in [15]. The basic algorithm for the spectrum modification in SANDPET is the same as in SAND-II.

The cross section library which is applied can be made from point cross section values with the program CSTAPE from the SAND-II program package. The program CSTAPE performs the interpolation and, if required, some extrapolations.

The program SAND-II can perform automatically corrections for the presence of foil covers during the irradiations. The cross sections of the cover materials have to be stored in a special section of the cross section library.

In the DOSCROS77 library cross section data for Au, B and Cd are available. The input data have to be given in a free format type, which is very useful in practice.

The speed of the convergence cannot be adjusted in the SAND-II program and is much dependent on the actual input, so no extra runs are required as for CRYSTAL BALL and RFSP-JÜL.

The input spectrum has to be supplied in the form of a series of point flux density values.

The program interpolates and can also extrapolate with various functions which can be selected.

An input spectrum is generated in 620 groups.

The convergence value, determined by the standard deviation of the ratio A_i^m / A_i^c , which is applied, is less favourable than the ARD criterion, especially if the input information comprises also uncertainties in SAND for the reaction rate data.

The average relative deviation as used in CRYSTAL BALL seems more suitable.

The computer memory needed by the program (SANDPET) is about 45 k.

A typical run with the program takes about 13 s.

A drawback of the program is that sometimes the changes in the A_i^m / A_i^c ratio become so small after some iterations, that the iterations are stopped and a so called "stability" is obtained before the required convergence criterion has been met. In this case too small modifications have to be expected.

3.4. STAY'SL | 10 |

Due to the extensive covariance matrix information required at the input of this program it was not easily and directly suitable for the unfolding problems of interest, but with some simplifying assumptions on the uncertainty of the input data some runs could be made. The only extra uncertainty which was required was the uncertainty of the input flux density values. These were taken equal for each of the 75 groups and the correlations of these values were assumed to be zero. The value of the uncertainties were selected in such a way that the ratios of input reaction rate and calculated reaction rate were comparable with those of the other programs (same value for the average relative deviation).

For the preparation of the input data a number of utility programs is required. These programs are not optimal at this moment and for this reason an input preparation requires much effort, especially if the number of groups has to be changed or if the reaction set is altered. A somewhat unpractical feature of the present version of STAY'SL is also that the reaction name is not printed directly, but has to be found from a sequence number. Up till now we did not improve the output features of the program.

The programs XCOV and FCOV prepare the cross section covariance matrix and the flux density covariance matrix, respectively. The number of elements in these matrices for a case of 75 groups and 20 reactions is $\approx 5.6 \times 10^3$ and $\approx 1.12 \times 10^5$, respectively for FCOV and XCOV.

In our study we had not enough detailed information on correlations between the group flux densities of the input spectrum. We assumed that all non-diagonal elements in the covariance matrix were zero, and that all diagonal elements were the same. This resulted in a rather small input for FCOV.

The input for XCOV contains zeroes for all matrix elements, which resulted also in a rather simple input deck.

When better covariance data for the cross section data file become available, an extra utility program will be required to determine the matrix of interest for a particular reaction set, which does not contain all reactions which are present for the cross section data file.

Due to the rather broad energy groups which have to be used, one has to apply well defined group cross sections.

These data can be calculated with the best estimate of the input spectrum and detailed cross section data.

Here a cross section library in the SAND-II format was applied.

Due to this procedure a clear correlation between the flux density data and the cross sections is introduced, which complicates the matter.

It is not yet clear how to avoid this pitfall, but, due to the crude selection of the cross section covariance file, this problem will not influence the results which are presented here.

The input data for the programs have to be given in a formatted form.

At present no provisions are available to take into account the possible presence of detector covers.

In principle no convergence criterion has to be applied in STAY'SL, but, due to lack of knowledge of the flux density uncertainty, some calculations with various flux density uncertainties were performed until an acceptable value for the ARD was obtained. This "misuse" of the program was required to obtain some data on the performance of STAY'SL.

Inconsistent input data sets are indicated in the program output.

The program STAY'SL is rather small; in our case it required ≈ 27 k memory positions. The typical calculation time for a run is about 3 s.

The plotting and other output treatment procedures have to be performed with a special output program.

A program which presents all data in a clear form is not yet available.

4. THE ACTUAL UNFOLDING PROCEDURE

In the preceding chapters the input data and the unfolding codes have been discussed. For a neutron spectrum calculation an input data set and an unfolding code is required. All the data are punched and an unfolding run is performed. The probability that already in the first run an acceptable output is obtained is quite small. In a number of cases this can be due to simple punching errors and clearly incorrect activity values. But even after correction of this type of mistakes problems often occur. This can be due to inconsistencies in the input data. These can be caused by an unfavourable or unrealistic choice of the input spectrum or by incorrect extrapolations of correct data. Another reason can be inconsistencies in the input- or the calculated reaction rate. It is also possible that too much structure is generated in the output spectrum (peaks and valleys, negative flux density values). In some cases, especially in fast neutron spectra, different reactions with similar response range tend to modify in an opposite way. This tendency may become apparent e.g. as local structure in the spectrum plots for SAND-II and CRYSTAL BALL, or as unrealistic small values of the ratio A_m/A_c for the other reactions in the output of RFSP-JÜL and STAY'SL.

The speed of convergence which is needed to obtain the correct convergence value in a suitable number of steps can only be determined by trial. If the code STAY'SL is applied, also several somewhat modified input data sets can be required to obtain an acceptable result. This is especially the case when the uncertainty data of the input spectrum data have to be estimated.

The problems mentioned above imply that the unfolding is not a straightforward procedure. Sometimes it is not easy to find the origin of an inconsistency in the input data set and to correct for it, because "trustworthy" data seem to be "suspected" in some cases.

In the following section some comment is given on the inconsistencies and what can be done to obtain consistent data.

4.1. Inconsistencies in the input data

The detection of reactions which show inconsistencies is for some unfolding codes rather difficult (RFSP-JUL, CRYSTAL BALL, and SAND-II), and rather easy for STAY'SL where a message is printed when the program discovers that the input deck contains unlikely information.

The ratio of input and calculated reaction rates of the other codes at the first iteration step may give a ratio which does not fit in the pattern of the other ratios, which may indicate an inconsistency. If an inconsistency is present in the input data, some action should follow.

Possible actions on the input data are:

- 1) Modification of the input spectrum;
- 2) Deletion of the suspected reaction from the input data;
- 3) For some unfolding codes an increase of the uncertainty data for the activity can be suitable.

If no extra information is available, we cannot give a preference rule for action.

4.1.1. Modification of the input spectrum

The modification of the input spectrum data is not possible if they have a good quality, but in several cases an extrapolation has to be performed, especially for the unfolding procedure. This extrapolation can refer to the fast part of the spectrum (fission or fusion) or to the low energy side where also various extrapolations can be made.

When the input spectrum information is available as group flux density values, an interpolation can be used to obtain a smooth spectrum without the block structure.

For a thermal reactor the thermal part of the neutron spectrum is important when activities induced by capture reactions play an important role. For this reason it is often useful to try several input spectra with various values for the matching constant μ determining the joining point $E = \mu kT$ between the Maxwellian and the $1/E$ distribution; also some change of the neutron temperature can be fruitful.

The best input spectrum can be determined on basis of the lowest deviations of input and calculated reaction rates or on basis of a smooth spectrum shape in the $1/E$ part.

On the high energy side of the spectrum also various versions of extrapolations can be tried, but in most cases this is not necessary, because

the modification information in this part of the neutron spectrum has a better quality, so that the role of the input spectrum is not so important in this energy region.

When the overall results of the unfolding are bad, it should be considered whether the best estimate applied for the neutron spectrum is still valid or whether it has to be updated. The selection of the input spectrum turns out to play an essential role in the unfolding procedure. When unfolding codes apply a limited number of groups, and the input spectrum consists also of a limited number of groups, then some precautions are necessary with respect to the preparation of the input spectrum (see 2.2.2.).

4.1.2. Deletion of a suspected reaction

Even after the best adjustment of the input spectrum it can happen that the results for one or a few reactions show clear inconsistencies with respect to the other reactions. This inconsistency can be seen from the difference of input and calculated reaction rates at the first iterations or from structure in the output spectrum which cannot be ascribed to the actual neutron field. The input data inconsistency has to be removed to obtain a more reliable output spectrum.

The modification of the input reaction set is complicated because:

- A real inconsistency can be present;
- Extreme or suspected values might however indicate extremely valuable information;
- The inconsistency is only available with respect to other "good" information.

For these reasons it is difficult to decide which is the origin of the inconsistency and to take proper measures.

If no explanation for the inconsistency can be found, the influence of the reaction on the unfolding process has to be reduced or the reaction has to be removed from the input data deck.

Improved results can also be obtained with an adapted convergence criterion, but in this case relatively small modifications will be obtained which can be effected strongly by suspected reactions.

4.1.3. Reduction of uncertainty

As described in 4.1.2 the inconsistencies can be removed by reducing the influence on the unfolding from the reaction which is suspected. This can be obtained by increasing the uncertainty data of the reaction of interest in the input deck. The amount of increase depends on the judgement of the unfolding physicist whether the reaction of interest should still have influence on the results or that the influence can be neglected.

4.2. Inconsistencies due to convergence criterion

For a good input data deck inconsistent results can be obtained if the unfolding procedure implies a too large modification. This can be due to a too pessimistic choice of the input spectrum uncertainties for STAY'SL or a too low convergence value for the other unfolding codes. The inconsistencies resulting from this source can be detected by inspecting the spectrum shape of the output spectrum.

Much structure, strong and physically unexpected strong changes, negative flux density points are illustrations of these inconsistencies.

This type of inconsistencies can be reduced by modification of the convergence conditions. Here also care is required because the actually applied criterion determines the degree of the modification and so the output spectrum.

4.3. Sources of inconsistencies

The sources of inconsistencies are in general related to the uncertainties in the input reaction rates or in the input cross section data.

Even a particular cross section set can show for various neutron spectra a different behaviour with respect to other reactions.

Due to lack of good uncertainty information this may lead to inconsistencies.

The experimental activity determination method can also lead to inconsistent activity data sets due to incorrect nuclear data or too large and unknown uncertainties of these data.

The nuclear data which are needed may comprise:

- The specific number of atoms of the sample;
- The half-life of the product nuclide;

- The gamma-ray abundances of the product nuclide;
- The neutron spectrum dependent fission yield;
- In some cases the product nuclide itself is not measured, but a radioactive daughter; here more nuclear data and uncertainties are introduced in the calculation of the reaction rate. The experimental procedure of activity determination will also contribute to the uncertainty.

Important contributions can be expected from the actual measurement and the data treatment procedure. Here also the absolute activity determination has to be considered.

The detector mass determination can give appreciable uncertainty contributions if very small samples are applied or if mixtures containing the detector material are applied.

Impurities in the detector material and contamination of the sample can lead to systematic errors. This type of errors is difficult to trace and has to be considered for each case separately.

The presence of strong cross section resonances in materials present in the irradiation surroundings can lead to inconsistencies if these resonances agree in energy with resonances in the detector set and if they are not taken into account in the input spectrum.

An unjustified input spectrum choice can also lead to inconsistencies which are difficult to detect.

4.4. Some experiences

Inconsistencies when they occur will lead in most cases to an iteration procedure in which the output of one calculation determines the composition of the new input deck. The steps which are needed in such a procedure depend on the actual situation and on the experience of the unfolding physicist. In some cases more than 20 runs were required to find the reason of an inconsistency.

The experience which is needed to obtain acceptable output spectra is difficult to describe. Experience with 10 collaborating guest scientists and students showed that the actual unfolding procedure did not give much problems, but that very often the handling of utility software gave lots of problems due to an unsatisfactory description of the program details, while also the preparation and adaptation of the input to correct for inconsistencies was rather time consuming. In most cases 3 months were required to obtain a good experience.

An unfolding code can never be used as a black box; a single run never guarantees an output spectrum which can be accepted as solution spectrum.

5. PRESENTATION OF THE RESULTS OF AN UNFOLDING PROCEDURE

For a good interpretation of the results it is required that each unfolding code gives the proper information. This information should contain the ratio of input and calculated activity for each input reaction.

If input values for reaction rate uncertainties are applied, it is also useful to give this ratio divided by this uncertainty value.

The output should also contain the standard deviation of all ratios and, if input uncertainties are applied, also the average relative deviation. The shape of the output spectrum should always be inspected by means of a plot with appropriate scales. In these plots structure can often be observed rather easily.

For thermal reactor neutron spectra the flux per unit lethargy can be plotted with much less decades on the flux density scale than if the flux per unit energy is plotted. The advantage is that irregularities are detected easier and faster.

It is often worthwhile to plot also the ratio of output and input spectrum. This ratio as a function of the energy shows often a more detailed picture of unfolding process than the output spectrum.

In a number of cases some extra information on the performance of a code can be obtained with a Monte Carlo error calculation or with an improvement ratio calculation. These data can also be plotted.

The spectrum information can also be printed and a conversion to broader energy groups facilitates the comparison with the calculated input spectrum sometimes. Also some characteristics of the spectra can be presented (i.e. the mean energy, etc.).

6. RESULTS

During the execution of the comparison of unfolding procedures several neutron spectra have been unfolded with the programs SAND-II, RFSP-JUL and CRYSTAL BALL, and in some cases with STAY'SL. The neutron spectra which were considered originated from fission sources, from accelerators, from fast reactor facilities, and from thermal reactors.

The input spectra which were used originated in most cases from physics calculations which resulted in a rather small number of groups.

In order to obtain comparable results for the programs with rather small and rather large number of groups, all input spectrum information was converted to smooth data in the SAND-II group structure. These smooth data were then converted to the coarser group structure.

6.1. No input weight data

A number of calculations has been performed with input data sets in which no activity uncertainties were applied. In this case the standard deviation of the ratios of the input reaction rate and the calculated reaction rate (as e.g. supplied by SAND-II) for the output spectrum seems a reasonable parameter to determine the convergence.

When no uncertainty information for the input data is available, then the value of this convergence parameter has to be estimated. In such an estimation not only the uncertainties of the reaction rates, but also the uncertainties in the calculated reaction rates due to cross section uncertainties should be taken into account.

In table 1 the uncertainties in typical reaction rates for several spectra are shown. The uncertainties in the experimental reaction rates are about 2½% for activation reactions, and 4 to 5% for fission reactions under favourable conditions. Combination of the two contributions gives the total uncertainty for the reaction of interest. The rounded average value of these uncertainties (which are assumed to have comparable values) is probably a good input value for the convergence parameter. A value lower than this estimate will lead to modification of the spectrum in a random way, dependent on the actual reaction rate value which is applied. A larger value will lead to a too small modification of the spectrum, and then good input information will not be used in an optimum way. The detection of inconsistencies in the input data is rather troublesome if no weight data are applied.

If too many reactions are deleted information is wasted; if inconsistent data are applied, a biased output spectrum will be obtained.

This dilemma leads to a subjective choice which may have a large influence on the shape of the output spectrum, and its characteristic properties. Typical results obtained with CRYSTAL BALL, RFSP-JÜL and SAND-II for the CFRMF spectrum are given in fig. 1, which shows the form of the ratio of output spectrum and input spectrum.

The input data are obtained from |16| and |5|.

In the calculations the reactions $^{238}\text{U}(n,\gamma)$, $^{45}\text{Sc}(n,\gamma)$, $^{115}\text{In}(n,\gamma)$, $^{47}\text{Ti}(n,p)$, $^{48}\text{Ti}(n,p)$ and $^{115}\text{In}(n,n')$ were not applied due to inconsistencies. From these results it follows that for the three programs applied, the contributions of fast neutrons in the energy region of 5 MeV is too small in the input spectrum. Also at about 10^{-4} MeV this effect seems to be present. This peak is due to the reaction $^{59}\text{Co}(n,\gamma)$. In the energy region between about 5×10^{-4} and 10^{-1} the modification of the three programs is different, but rather small in amplitude.

The program SAND-II gives a structure with sharp peaks and valleys.

The program CRYSTAL BALL gives a more smooth modification.

RFSP-JÜL seems also to give a smooth output spectrum, but this is partly due to the small number of groups. The modification pattern is characteristic for the code applied, but this holds not completely for STAY'SL, because the modification pattern of STAY'SL depends of course on the flux density covariance matrix.

Some characteristic modification patterns are shown in fig. 2 for a STEK fast neutron spectrum and only two reactions: one thermal activation reaction, $^{59}\text{Co}(n,\gamma)$, and one threshold reaction, $^{58}\text{Ni}(n,p)$. The step modification of SAND-II, the linearly changing modification of CRYSTAL BALL and the response dependent modifications of RFSP-JÜL and STAY'SL are clear. The flux density correlations between the various groups were assumed to be zero in the STAY'SL calculation.

In fig. 3 STAY'SL output spectra for the same input data are supplied with different covariance matrices. These results show that for STAY'SL the modification pattern $\phi_{\text{out}}/\phi_{\text{in}}$ is not a characteristic of the algorithm, but for the covariance matrix. These matrices can be chosen in such a way, that the modification pattern is similar to that of one of the other three codes.

In a series of calculations it was tried to remove the structure in the SAND-II output spectra by applying the smoothing procedure during the

unfolding calculations. The results were not really better and for this reason the smooth procedure was not applied in the actual unfolding calculations, see fig. 4.

Some results of three unfolding programs for a thermal reactor neutron spectrum (the LFR at Petten) are shown in figs. 5 and 6.

In some figures also the 90% response regions are indicated (5% of response below this region and 5% above).

Some of the detectors were irradiated under cadmium or boron covers to shift the response to higher energies, but even with these covers no appreciable response occurs between about 10^{-2} and 1 MeV.

The plots of the energy dependence of the $\phi_{\text{out}}/\phi_{\text{in}}$ ratio show that the overall tendency of the modification introduced by the three codes is approximate the same; the SAND-II program gives some detailed local structure, which is absent in case of CRYSTAL BALL.

6.2. With input weight data

Also calculations have been performed in which statistical weights for the reactions were applied; these weight factors were based upon values of the reaction rate uncertainties, specified at the input. The values applied were the square roots from the sum of the squares of the experimental uncertainty of the experimental reaction rate and of the estimated uncertainty in the calculated reaction rate (mainly based on cross section uncertainties).

Results which were obtained for the CFRMF neutron spectrum are presented in tables 2, 3 and 4 and figs. 7 and 8.

Table 2 shows the ratio and the relative ratio (with respect to reaction rate uncertainty) for the CFRMF input spectrum. From this table it follows that the 620 groups flux density spectrum results (obtained with CRYSTAL BALL and SANDPET) deviate clearly from the results for a 75 groups spectrum (obtained with RFSP-JUL and STAY'SL). The results for these latter two codes show also some clear deviations. These differences are due to loss of (real or putative) information in the conversion of the 620 groups spectrum to the 75 groups spectrum (see table 5 for the influence of this effect).

Two series of output spectra have been calculated for the four codes. First an average relative deviation equal to the uncertainty was applied; this yielded a "too good" output spectrum. Good output spectra were

obtained for an average relative deviation of about 1.45. The results are shown in table 4 and in figs. 7 ... 9.

Especially fig. 9 shows the effects of a "too good" output spectrum (obtained for an average relative deviation of about 1) in the energy region of about 10^{-2} MeV: A rather wide valley in the CRYSTAL BALL output, much structure in the SANDPET output, and a rather narrow valley for RFSP-JÜL and STAY'SL.

The results presented in figs. 7 and 8 show the output spectrum results which are accepted as a reasonable output. The spectrum shape is rather smooth (fig. 7).

The ratio of output and input spectrum shows for all programs the same type of modification between 10^0 and 10^1 MeV, at about 10^{-2} MeV, and at about 10^{-4} MeV. The CRYSTAL BALL output ratio is probably too smooth and the structure in the SANDPET results is not likely to occur in the actual neutron spectrum.

The valleys in fig. 8 are due to the reaction $^{238}\text{U}(n,\gamma)$. Probably the information of this reaction is not consistent with the other reaction data. The output spectrum data of RFSP-JÜL and STAY'SL does not have enough information to decide on inconsistencies, but the peak at about 10^{-4} MeV and the two valleys just beside it are rather pronounced. At this point the decision to accept the output or to go on without the $^{233}\text{U}(n,\gamma)$ reaction (or with an adjusted uncertainty) and probably also a smaller convergence value can be made. For this example no further calculations have been done. Some additional calculations resulted in the improvement ratios, see fig. 10. The programs CRYSTAL BALL and SANDPET show in this figure a valley in the energy region between about 10^{-1} and 10^0 MeV. In this region, where there is no appreciable detector response, the codes show, as we have seen in the case of only two detectors, typical different modification behaviour. Because of the low value of the improvement ratio, however, no real improvement can be expected in this energy region. The same is valid for the codes RFSP-JÜL and STAY'SL, but these codes do not modify when the response is small, so no real modifications can be expected (STAY'SL did not use correlation data for the input flux density values in this calculation).

In fig. 11 the results of a Monte Carlo calculation with SANDPET are shown. In this figure we observe that the magnitude of the uncertainty of the output spectrum is quite large, not only in the energy region (0.1 to 1 MeV), where detector response is poor, but also in the region between

1 and 5 MeV. In the keV region we observe too much structure in the solution, accompanied by large uncertainties. The uncertainty in the output spectrum is mainly determined by the uncertainty values for the cross section data, and to a lesser extent by the uncertainty value of the reaction rate data.

7. CONCLUSION

From the results which are presented for the set of input data applied here it follows that the four unfolding codes give comparable output spectra if a number of precautions in preparing the input data is taken into account.

Important aspects for the actual unfolding procedure are:

- The conversion of the input flux density values;
- The determination of the input uncertainty (combination of input reaction rate and calculated reaction rate uncertainty for the input spectrum);
- The choice of a suitable convergence value;
- The detection of inconsistencies in the input data.

The first two subjects can be solved quite easily, the two following aspects are more difficult to handle in an objective way. This is due to a too limited knowledge on the quality of the input data (i.e. cross sections and reaction rate data). For this reason no optimal results may be expected for neutron spectrum unfolding without improved input data information. The improved input data should comprise at least:

- A consistent cross section library with uncertainty data;
- Detailed input spectrum data and, if possible, also uncertainty data;
- A consistent input reaction set with uncertainties. Consistent means that no reactions have to be deleted during the unfolding calculations;
- More experimental data in important neutron spectrum regions (for damage predictions the energy region between 10^{-2} and 1 MeV). Also the energy region from 10^{-6} to 10^{-2} MeV needs more experimental information.

All uncertainty data should, if possible, include both variances and covariances. If all this information is available, the program STAY'SL can give good results.

In the case that inconsistencies can be expected the program SANDPET is convenient to show them by means of local structure in the plot of the output spectra.

Under favourable conditions the other programs will yield comparable results.

The quality of the input data and the output data should always be judged from a physics point of view.

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Table 1. Uncertainties in calculated reaction rates.

Values (in %) are based upon cross section data in the DOSCROS77 library [2], and upon the SAND-II cross section error library [5].

reaction	neutron spectrum			
	LFER	CFRMF	²⁵² Cf	TOKOMAK
⁶ Li(n,α) ³ H	0.49	6.43	6.17	5.16
¹⁰ B(n,α) ⁷ Li	0.49	3.85	6.22	3.42
²³ Na(n,γ) ²⁴ Na	0.98	5.63	4.29	6.11
²⁴ Mg(n,p) ²⁴ Na	6.46	6.46	6.40	9.33
²⁷ Al(n,α) ²⁴ Na	3.92	3.91	3.88	9.39
²⁷ Al(n,p) ²⁷ Mg	3.78	3.79	3.80	16.83
³¹ P(n,p) ³¹ Si	6.43	5.49	5.27	6.74
³² S(n,p) ³² P	7.64	6.11	5.40	5.80
⁴⁵ Sc(n,γ) ⁴⁶ Sc	1.96	5.12	5.32	5.14
⁴⁶ Ti(n,p) ⁴⁶ Sc	7.69	7.51	7.43	17.50
⁴⁷ Ti(n,p) ⁴⁷ Sc	13.80	12.39	11.12	11.80
⁴⁸ Ti(n,p) ⁴⁸ Sc	8.86	8.87	8.75	14.34
⁵⁴ Fe(n,p) ⁵⁴ Mn	3.82	3.84	3.77	7.17
⁵⁵ Mn(n,γ) ⁵⁶ Mn	0.81	6.37	4.82	6.66
⁵⁶ Fe(n,p) ⁵⁶ Mn	3.64	3.67	3.66	13.99
⁵⁸ Fe(n,γ) ⁵⁹ Fe	7.63	15.04	6.46	14.61
⁵⁸ Ni(n,2n) ⁵⁷ Ni	19.59	19.59	19.63	20.00
⁵⁸ Ni(n,p) ⁵⁸ Co	2.30	2.24	2.24	6.89
⁵⁹ Co(n,γ) ⁵⁶ Mn	5.97	5.98	5.92	9.52
⁵⁹ Co(n,γ) ⁶⁰ Co	3.73	8.55	4.81	8.90
⁶⁰ Ni(n,p) ⁶⁰ Co	6.12	6.13	6.08	8.90
⁶³ Cu(n,α) ⁶⁰ Co	6.36	6.37	6.31	9.16
⁶³ Cu(n,2n) ⁶² Cu	6.06	6.06	6.14	7.97
⁶³ Cu(n,γ) ⁶⁴ Cu	4.75	5.89	4.60	5.71
⁶⁴ Zn(n,p) ⁶⁴ Cu	11.63	11.01	9.97	11.13
⁹⁰ Zr(n,2n) ⁸⁹ Zr	13.53	13.53	13.58	14.98
¹⁰⁹ Ag(n,γ) ¹¹⁰ Ag	1.96	4.97	4.32	4.99
¹¹⁵ In(n,n) ¹¹⁵ In	5.76	5.54	4.49	4.12
¹¹⁵ In(n,γ) ¹¹⁶ In ^m	2.59	2.77	5.59	2.78
¹²⁷ I(n,2n) ¹²⁶ I	17.66	17.66	17.33	14.68
¹⁹⁷ Au(n,γ) ¹⁹⁸ Au	1.55	3.16	3.21	3.21
²³² Th(n,f)FP FP	11.84	9.45	8.18	8.15
²³² Th(n,γ) ²³³ Th	2.73	4.21	4.86	4.42
²³⁵ U(n,f)FP FP	0.50	3.54	2.11	3.77
²³⁷ Np(n,f)FP FP	3.04	3.83	1.92	5.86
²³⁸ U(n,f)FP	2.42	2.15	1.70	7.74
²³⁸ U(n,γ) ²³⁹ U	3.93	4.26	4.16	4.57
²³⁹ Pu(n,f)FP	0.50	3.48	2.31	3.78

Table 2. Values for A_m/A_c and $(A_m - A_c)/s(A_m - A_c)$ for the CFRMF input spectrum.

reaction	A_m/A_c				$A_m - A_c$ divided by uncertainty			
	CRYSTAL BALL	RFSP-JÜL	SANDPET	STAY'SL	CRYSTAL BALL	RFSP-JÜL	SANDPET	STAY'SL
$^{27}\text{Al}(n,\alpha)^{24}\text{Na}$	0.9032	0.9201	0.9032	0.9210	-3.78	-1.86	-3.78	-1.83
$^{27}\text{Al}(n,p)^{27}\text{Mg}$	0.9560	0.9778	0.9560	0.9741	-0.98	-0.49	-0.98	-0.57
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	1.1523	1.1896	1.1523	1.1736	5.41	3.39	5.41	3.09
$^{46}\text{Ti}(n,p)^{46}\text{Sc}$	1.1104	1.1348	1.1104	1.1325	2.16	1.71	2.16	1.68
$^{48}\text{Ti}(n,p)^{48}\text{Sc}$	1.0107	1.0305	1.0107	1.0307	0.14	0.33	0.14	0.33
$^{47}\text{Ti}(n,p)^{47}\text{Sc}$	0.8893	0.9070	0.8893	0.9057	-2.92	-0.71	-2.92	-0.72
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	1.0381	1.0607	1.0381	1.0576	0.48	1.45	0.48	1.37
$^{58}\text{Fe}(n,\gamma)^{59}\text{Fe}$	0.9676	1.0064	0.9676	0.9857	-0.35	-0.04	-0.35	-0.09
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	1.0771	1.0997	1.0771	1.0973	0.83	3.56	0.83	3.46
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	1.1500	1.0345	1.1500	1.1687	1.99	0.38	1.99	1.88
$^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$	0.9423	0.9769	0.9423	0.9605	-1.43	10.31	-1.43	-0.52
$^{115}\text{In}(n,n')^{115}\text{In}$	1.0808	1.1011	1.0808	1.1006	0.61	1.40	0.61	1.39
$^{115}\text{In}(n,\gamma)^{116}\text{In}^m$	0.9239	0.9469	0.9239	0.9407	-2.11	-1.33	-2.11	-1.48
$^{197}\text{Au}(n,\gamma)^{198}\text{Au}$	1.0123	1.0292	1.0123	1.0317	0.32	0.81	0.32	0.88
$^{235}\text{U}(n,f)\text{FP}$	0.9664	0.9911	0.9664	0.9852	-0.78	-0.23	-0.78	-0.38
$^{237}\text{Np}(n,f)\text{FP}$	0.9888	1.0138	0.9888	1.0079	-0.19	0.31	-0.19	0.17
$^{238}\text{U}(n,f)\text{FP}$	1.0655	1.0863	1.0655	1.0869	1.56	3.36	1.56	3.33
$^{238}\text{U}(n,\gamma)^{239}\text{U}$	0.7726	0.7909	0.7726	0.7871	-1.49	-4.11	-1.49	-4.18
$^{239}\text{Pu}(n,f)\text{FP}$	0.9926	1.0183	0.9926	1.0114	-0.16	0.48	-0.16	0.30
ARD	1.93	1.54	1.93	1.94	1.93	1.54	1.93	1.94

Table 3. Values for A_m/A_c for the CFRMF solution spectrum.

reaction	A_m/A_c			
	CRYSTAL BALL	RFSP-JÜL	SANDPET	STAY'SL
$^{27}\text{Al}(n,\alpha)^{24}\text{Na}$	0.9904	0.9580	0.9334	0.9611
$^{27}\text{Al}(n,p)^{27}\text{Mg}$	0.9573	0.9576	0.9425	0.9575
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	1.2080	1.2049	1.1676	1.1903
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	0.9824	0.9973	1.0042	0.9982
$^{58}\text{Fe}(n,\gamma)^{59}\text{Fe}$	1.0051	1.0236	1.0144	1.0064
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	1.0198	1.0296	1.0405	1.0313
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	1.1242	1.0134	1.0579	1.0644
$^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$	0.9931	0.9996	0.9815	0.9905
$^{115}\text{In}(n,\gamma)^{116}\text{In}^m$	0.9731	0.9650	0.9528	0.9627
$^{197}\text{Au}(n,\gamma)^{198}\text{Au}$	1.0705	1.0502	1.0418	1.0544
$^{235}\text{U}(n,f)\text{FP}$	1.0060	1.0035	0.9892	1.0016
$^{237}\text{Np}(n,f)\text{FP}$	0.9915	0.9967	0.9847	0.9985
$^{238}\text{U}(n,f)\text{FP}$	1.0000	1.0027	1.0252	1.0062
$^{238}\text{U}(n,\gamma)^{239}\text{U}$	0.8194	0.8105	0.8148	0.8115
$^{239}\text{Pu}(n,f)\text{FP}$	1.0360	1.0276	1.0120	1.0250
$^{115}\text{In}(n,n')^{115}\text{In}^m$	1.0257	1.0309	1.0472	1.0356
$^{46}\text{Ti}(n,p)^{46}\text{Sc}$	1.1125	1.1115	1.0940	1.1129
$^{48}\text{Ti}(n,p)^{48}\text{Sc}$	1.0967	1.0642	1.0385	1.0668
$^{47}\text{Ti}(n,p)^{47}\text{Sc}$	0.8375	0.8451	0.8579	0.8472
ARD	1.46	1.46	1.47	1.45

Table 4. Values for $(A_m - A_c)/s(A_m - A_c)$ for two CFRFM output spectra.

reaction	output spectrum (ARD \approx 1.45)				too good output spectrum (ARD \approx 1.00)			
	CRYSTAL BALL	RFSP-JÜL	SANDPET	STAY'SL	CRYSTAL BALL	RFSP-JÜL	SANDPET	STAY'SL
$^{27}\text{Al}(n,\alpha)^{24}\text{Na}$	-0.22	-0.98	-1.54	-0.90	-0.22	-0.23	-0.35	-0.28
$^{27}\text{Al}(n,p)^{27}\text{Mg}$	-0.95	-0.94	-1.28	-0.94	-0.77	-0.84	-1.19	-0.83
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	3.70	3.66	2.98	3.39	1.53	1.99	1.73	1.85
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	-0.42	-0.06	0.10	-0.04	-0.42	0.26	-0.33	-0.23
$^{58}\text{Fe}(n,\gamma)^{59}\text{Fe}$	0.03	0.16	0.09	0.04	-0.05	0.10	0.27	0.02
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	0.70	1.05	1.44	1.11	0.46	0.68	0.67	0.70
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	1.38	0.15	0.64	0.71	0.35	-0.02	-0.01	0.03
$^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$	-0.09	0.00	-0.24	-0.12	-0.44	0.03	0.01	0.00
$^{115}\text{In}(n,\gamma)^{116}\text{In}^m$	-0.67	-0.88	-1.18	-0.93	-0.27	-0.52	-0.78	-0.52
$^{198}\text{Au}(n,\gamma)^{198}\text{Au}$	1.96	1.40	1.16	1.51	1.73	1.57	0.81	1.33
$^{235}\text{U}(n,f)\text{FP}$	0.15	0.09	-0.28	0.04	0.05	-0.09	-0.05	-0.04
$^{237}\text{Np}(n,f)\text{FP}$	-0.19	-0.07	-0.34	-0.03	0.06	0.21	-0.26	0.13
$^{238}\text{U}(n,f)\text{FP}$	0.00	0.11	0.98	0.24	-0.16	-0.15	-0.10	-0.11
$^{238}\text{U}(n,\gamma)^{239}\text{U}$	-3.54	-3.72	-3.63	-3.70	-2.60	-2.45	-2.47	-2.28
$^{239}\text{Pu}(n,f)\text{FP}$	0.95	0.73	0.31	0.66	0.70	0.42	0.52	0.44
$^{115}\text{In}(n,n')^{115}\text{In}^m$	0.35	0.43	0.65	0.49	0.44	0.39	0.35	0.37
$^{46}\text{Ti}(n,p)^{46}\text{Sc}$	1.42	1.41	1.19	1.43	1.42	1.35	1.23	1.31
$^{48}\text{Ti}(n,p)^{48}\text{Sc}$	1.05	0.70	0.41	0.72	0.76	0.98	0.95	0.93
$^{47}\text{Ti}(n,p)^{47}\text{Sc}$	-1.24	-1.18	-1.08	-1.17	-1.27	-1.25	-1.24	-1.24
ARD	1.46	1.46	1.47	1.45	1.01	1.02	0.995	0.959

Table 5. Influence of group structure for CFRMF spectrum.

The following notation is used:

- $\langle\sigma\rangle^{620}$ = the cross section averaged over the spectrum in its 620 group representation;
- $\langle\sigma\rangle^{75G}$ = the cross section averaged over the spectrum determined by 75 group values (spectrum is stepwise constant in E); this spectrum was obtained by simple condensation from the 620 group data ($\phi_E = \phi_g/\Delta E$);
- $\langle\sigma\rangle^{75P}$ = the cross section averaged over the spectrum, determined by 75 point values (spectrum is piecewise linear in E between the point values; $E = E/\Delta u$; $\phi_E = \phi_g/\Delta E$).

reaction	$\langle\sigma\rangle^{620}$ 1)	$\langle\sigma\rangle^{75G}/\langle\sigma\rangle^{620}$ 2)	$\langle\sigma\rangle^{75P}/\langle\sigma\rangle^{620}$ 3)
$^{27}\text{Al}(n,\alpha)^{24}\text{Na}$	$1.763 \cdot 10^{-28}$	1.033	1.004
$^{27}\text{Al}(n,p)^{27}\text{Mn}$	$9.004 \cdot 10^{-28}$	1.028	1.002
$^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}$	$2.007 \cdot 10^{-26}$	0.971	0.998
$^{46}\text{Ti}(n,p)^{46}\text{Sc}$	$2.315 \cdot 10^{-27}$	1.027	1.001
$^{48}\text{Ti}(n,p)^{48}\text{Sc}$	$6.710 \cdot 10^{-29}$	1.032	1.003
$^{47}\text{Ti}(n,p)^{47}\text{Sc}$	$4.624 \cdot 10^{-27}$	1.038	1.002
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	$1.655 \cdot 10^{-26}$	1.030	1.002
$^{58}\text{Fe}(n,\gamma)^{59}\text{Fe}$	$6.230 \cdot 10^{-27}$	0.982	1.007
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	$2.200 \cdot 10^{-26}$	1.035	1.002
$^{59}\text{Co}(n,\gamma)^{60}\text{Co}$	$7.846 \cdot 10^{-26}$	1.028	1.044
$^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$	$4.755 \cdot 10^{-26}$	0.996	1.002
$^{115}\text{In}(n,n\gamma)^{115}\text{In}^m$	$4.534 \cdot 10^{-26}$	1.055	1.008
$^{115}\text{In}(n,\gamma)^{116}\text{In}$	$3.006 \cdot 10^{-25}$	0.983	1.000
$^{197}\text{Au}(n,\gamma)^{198}\text{Au}$	$4.138 \cdot 10^{-25}$	0.976	0.997
$^{235}\text{U}(n,f)\text{FP}$	$1.588 \cdot 10^{-25}$	0.991	0.999
$^{237}\text{Np}(n,f)\text{FP}$	$5.493 \cdot 10^{-25}$	1.044	1.005
$^{238}\text{U}(n,f)\text{FP}$	$6.984 \cdot 10^{-26}$	1.052	1.007
$^{238}\text{U}(n,\gamma)^{239}\text{U}$	$2.343 \cdot 10^{-25}$	0.986	1.017
$^{239}\text{Pu}(n,f)\text{FP}$	$1.770 \cdot 10^{-24}$	0.999	0.999

1) $\langle\sigma\rangle^{620} = \sum_{i=1}^{621} \sigma^i(E) \cdot \phi_E^i(E) \Delta E^i / \sum_{i=1}^{621} \phi_E^i(E) \cdot \Delta E^i$
with $\phi_E(E)$ is the CFRMF spectrum

2) $\langle\sigma\rangle^{75G}$ = as above with $\phi_E(E)$ is the CFRMF spectrum (in 620 groups), converted to a histogram in 75 groups. The energy boundaries are shown in table 6; in each group $\phi_E(E)$ is constant; $\phi_E(E) = \phi_g/\Delta E$.

3) $\langle\sigma\rangle^{75P}$ = as above with $\phi_E(E)$ is the CFRMF spectrum, converted to a 75 point structure with $E = \Delta E/\Delta u$ and $\phi_E = \phi_g/\Delta E$; ΔE = width of the groups:

**Table 6. Boundaries of the energy structure in 75 groups
(expressed in MeV).**

0.100 10 ⁻⁹	0.210 10 ⁻¹	6.40
0.270 10 ⁻⁵	0.270 10 ⁻¹	6.90
0.960 10 ⁻⁵	0.360 10 ⁻¹	7.40
0.210 10 ⁻⁴	0.475 10 ⁻¹	7.90
0.475 10 ⁻⁴	0.600 10 ⁻¹	8.40
0.960 10 ⁻⁴	0.760 10 ⁻¹	8.90
0.120 10 ⁻³	0.960 10 ⁻¹	9.40
0.160 10 ⁻³	0.120	9.40
0.210 10 ⁻³	0.160	10.4
0.270 10 ⁻³	0.210	10.9
0.360 10 ⁻³	0.270	11.4
0.475 10 ⁻³	0.360	11.9
0.600 10 ⁻³	0.475	12.4
0.760 10 ⁻³	0.600	12.9
0.960 10 ⁻³	0.760	13.4
0.120 10 ⁻²	0.960	13.9
0.160 10 ⁻²	1.40	14.4
0.210 10 ⁻²	1.90	14.9
0.270 10 ⁻²	2.40	15.4
0.360 10 ⁻²	2.90	15.9
0.475 10 ⁻²	3.40	16.4
0.600 10 ⁻²	3.90	16.9
0.760 10 ⁻²	4.40	17.4
0.960 10 ⁻²	4.90	18.0
0.120 10 ⁻¹	5.40	
0.160 10 ⁻¹	5.90	

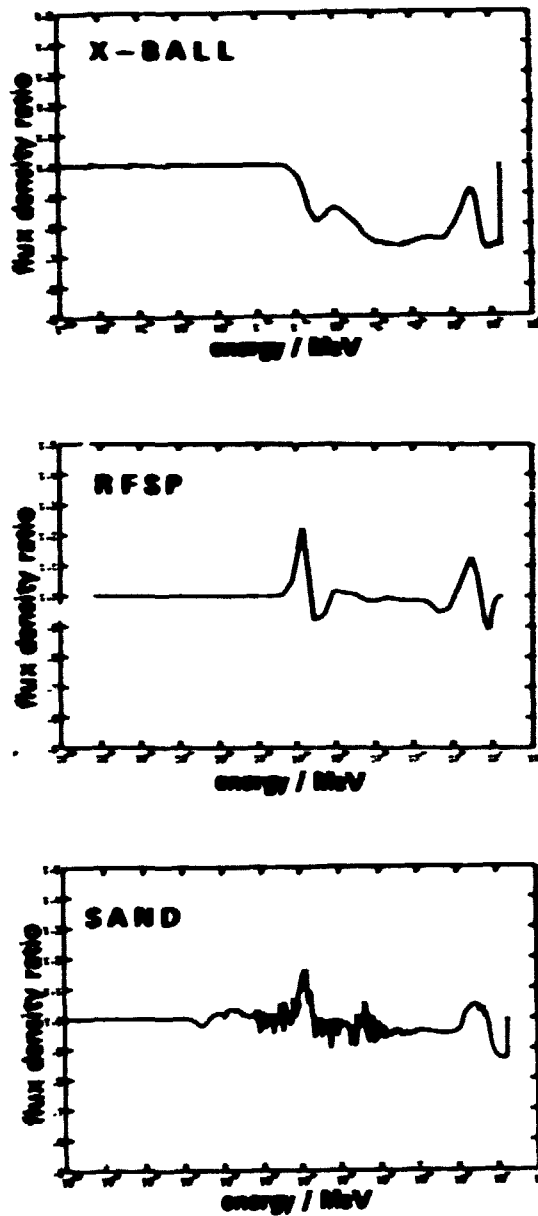


Fig. 1. Ratio of output and input spectrum calculated without uncertainty data for the CFFIF.

The ENDF/B-IV cross section library was used in these calculations.

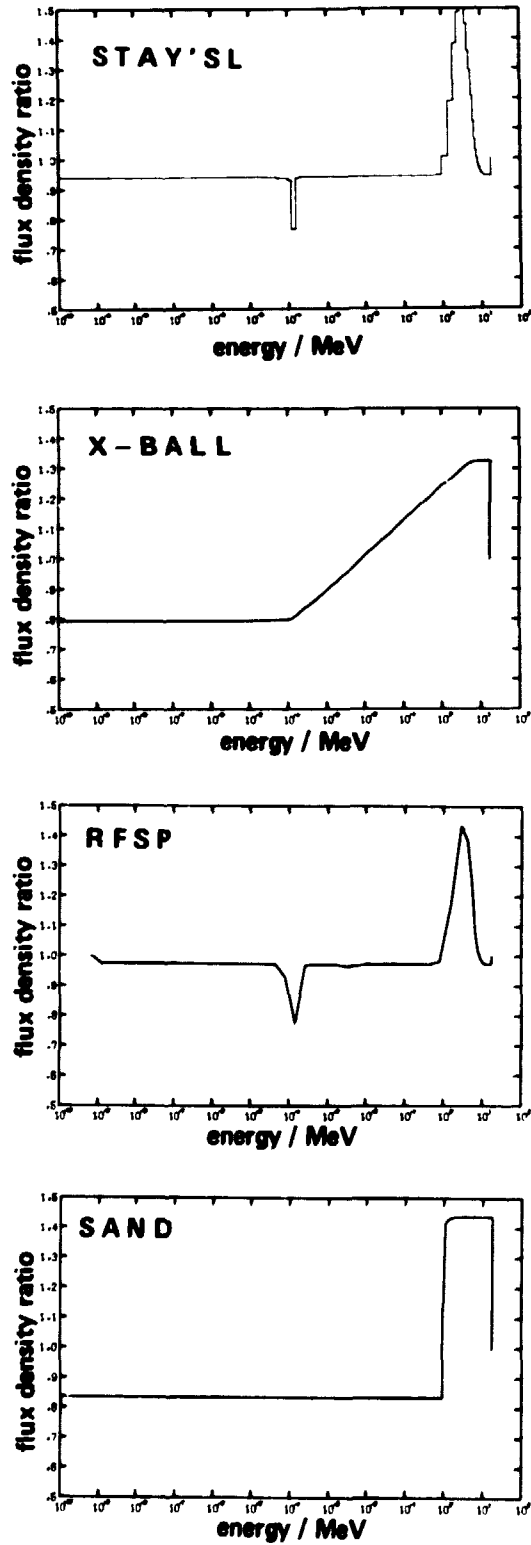


Fig. 2. Characteristic modification pattern.

Results for the Co and Ni set in a STEK spectrum.

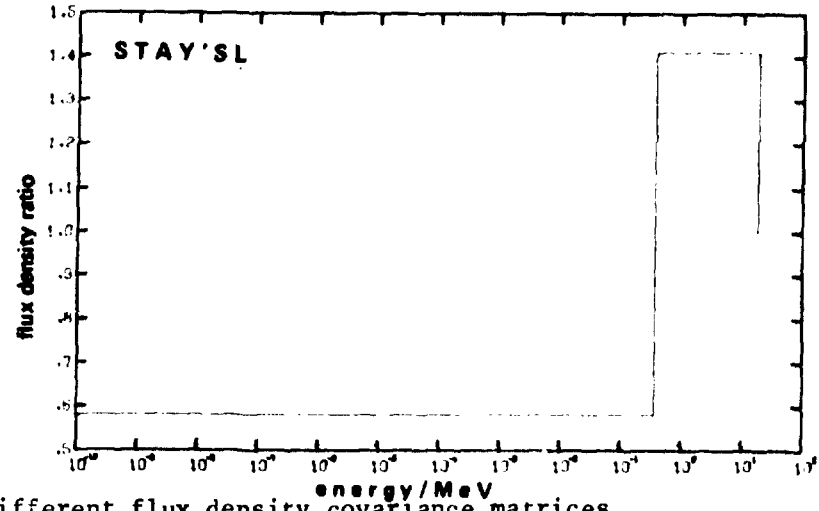
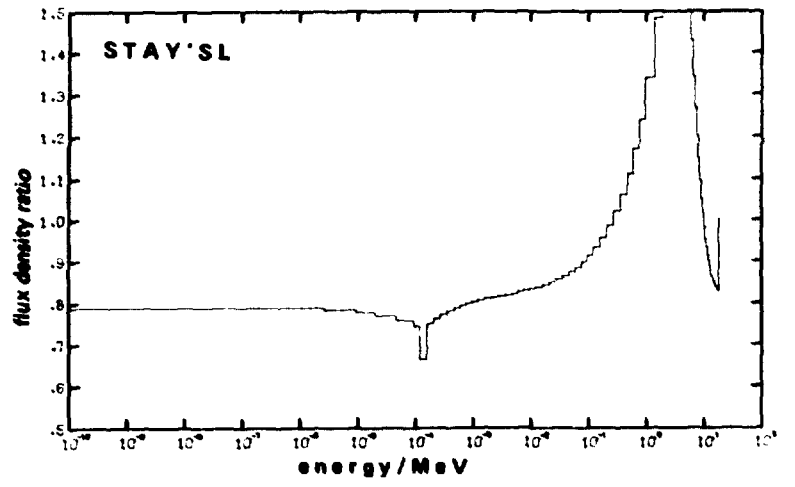
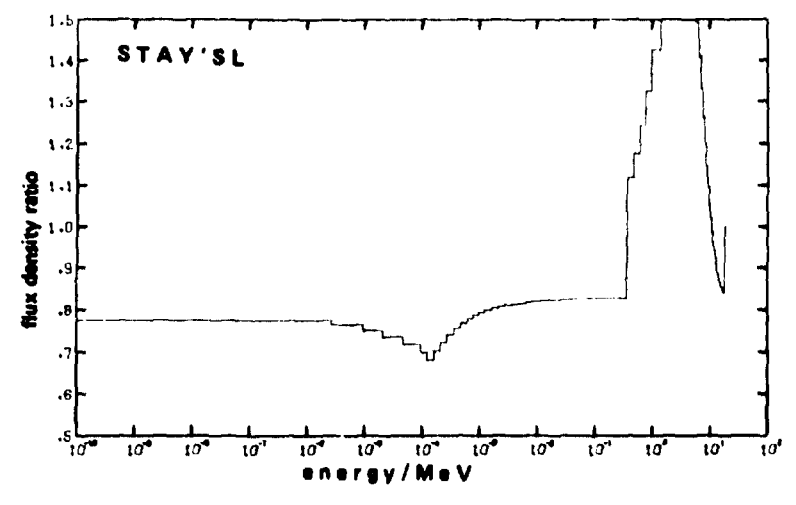
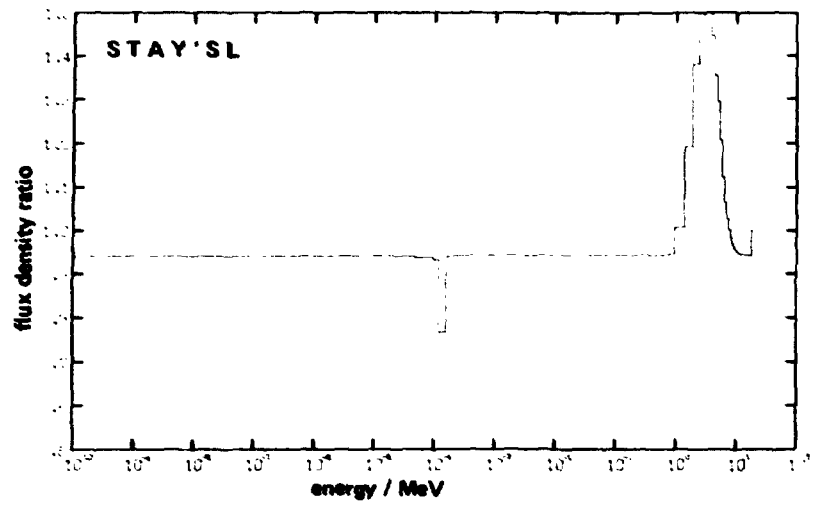


Fig. 3. Modification patterns for different flux density covariance matrices.
 Results for STAY'SL for the Co and Ni set in a STEK spectrum.

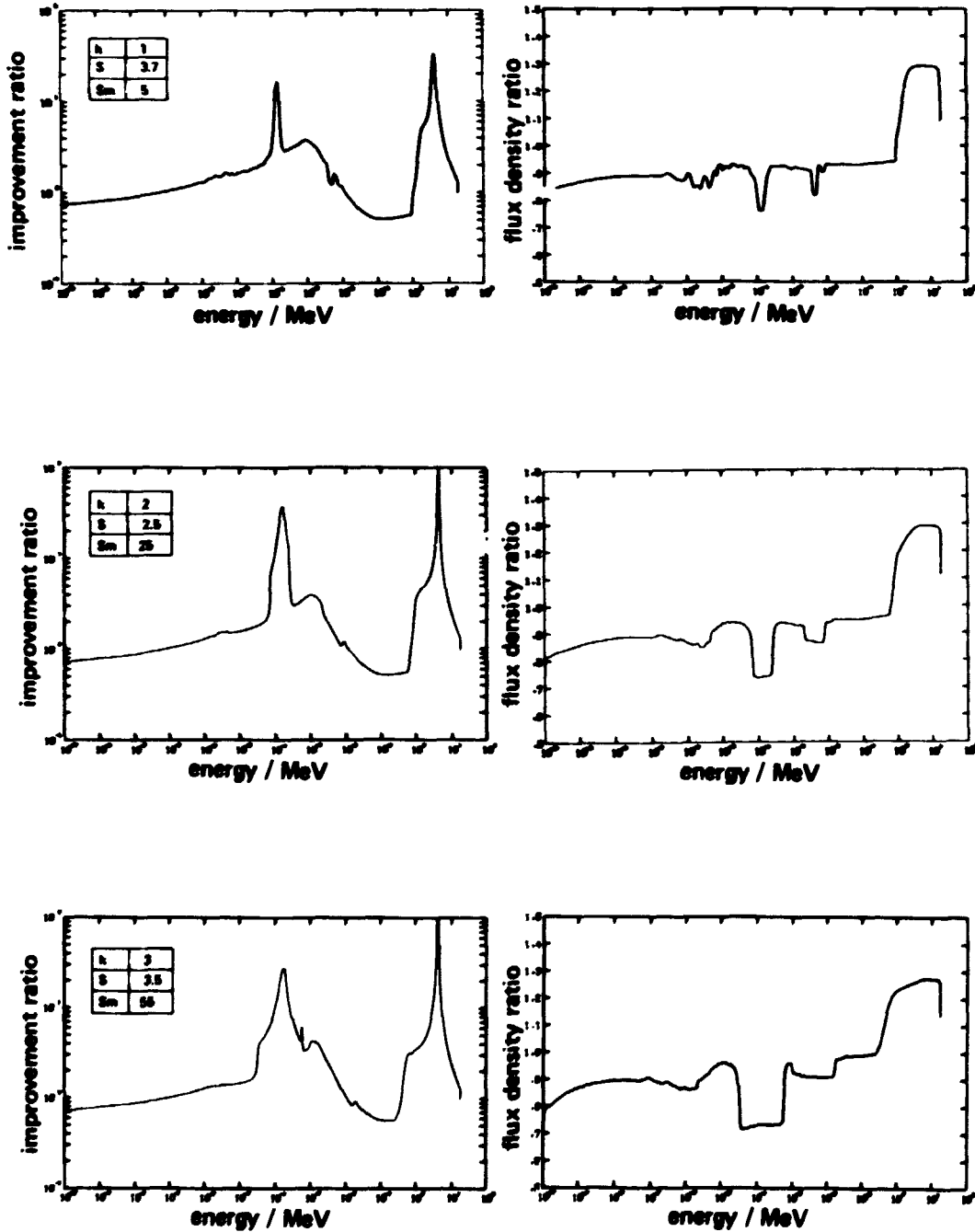


Fig. 4. Influence of smoothing in SAND-II.

K = number of iterations;
 σ = standard deviation of A^m/A^c values;
 S_m = number of groups used in smoothing.

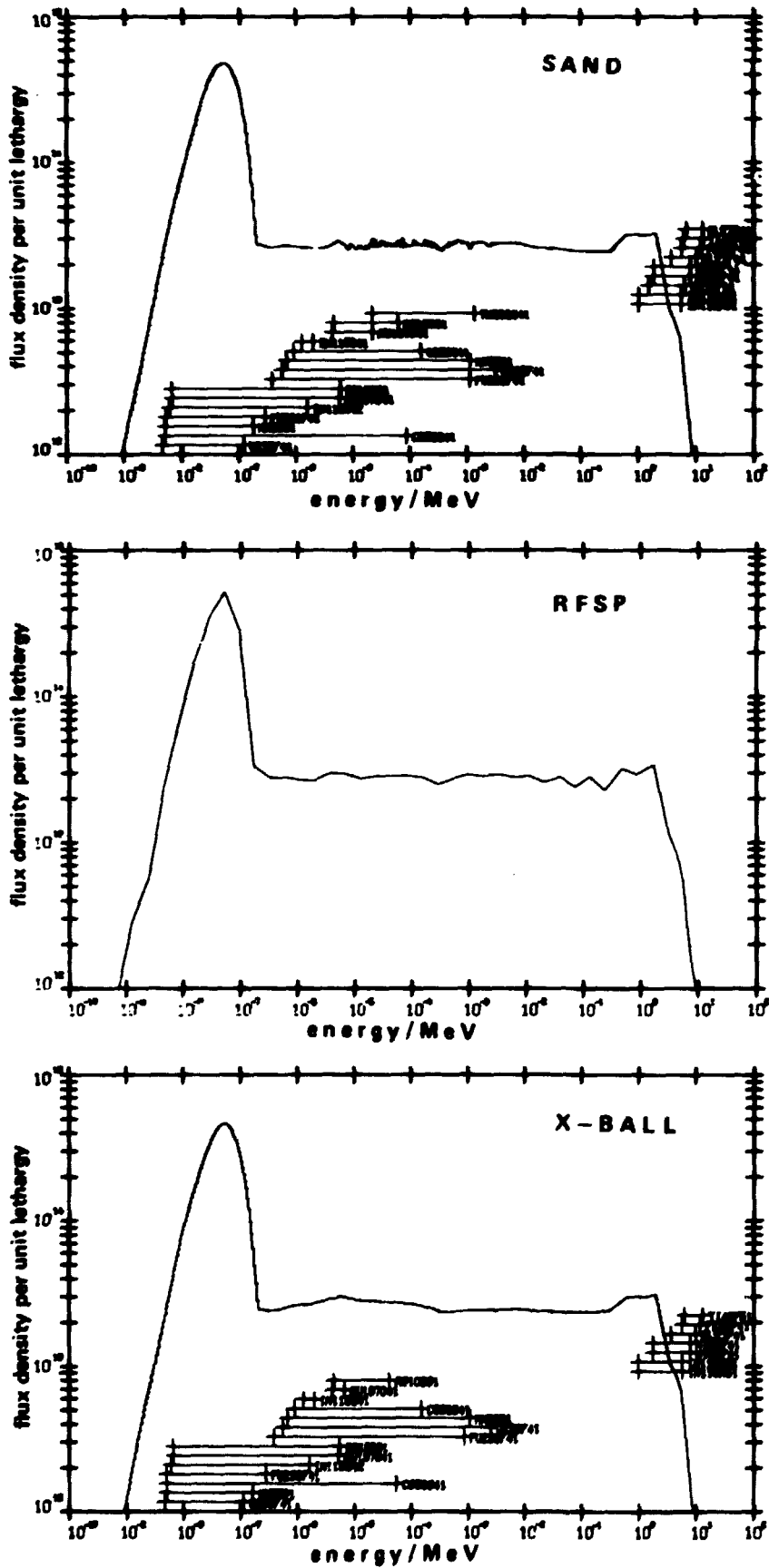


Fig. 5. Neutron spectra in the VC of the LFR calculated by the various unfolding programs.

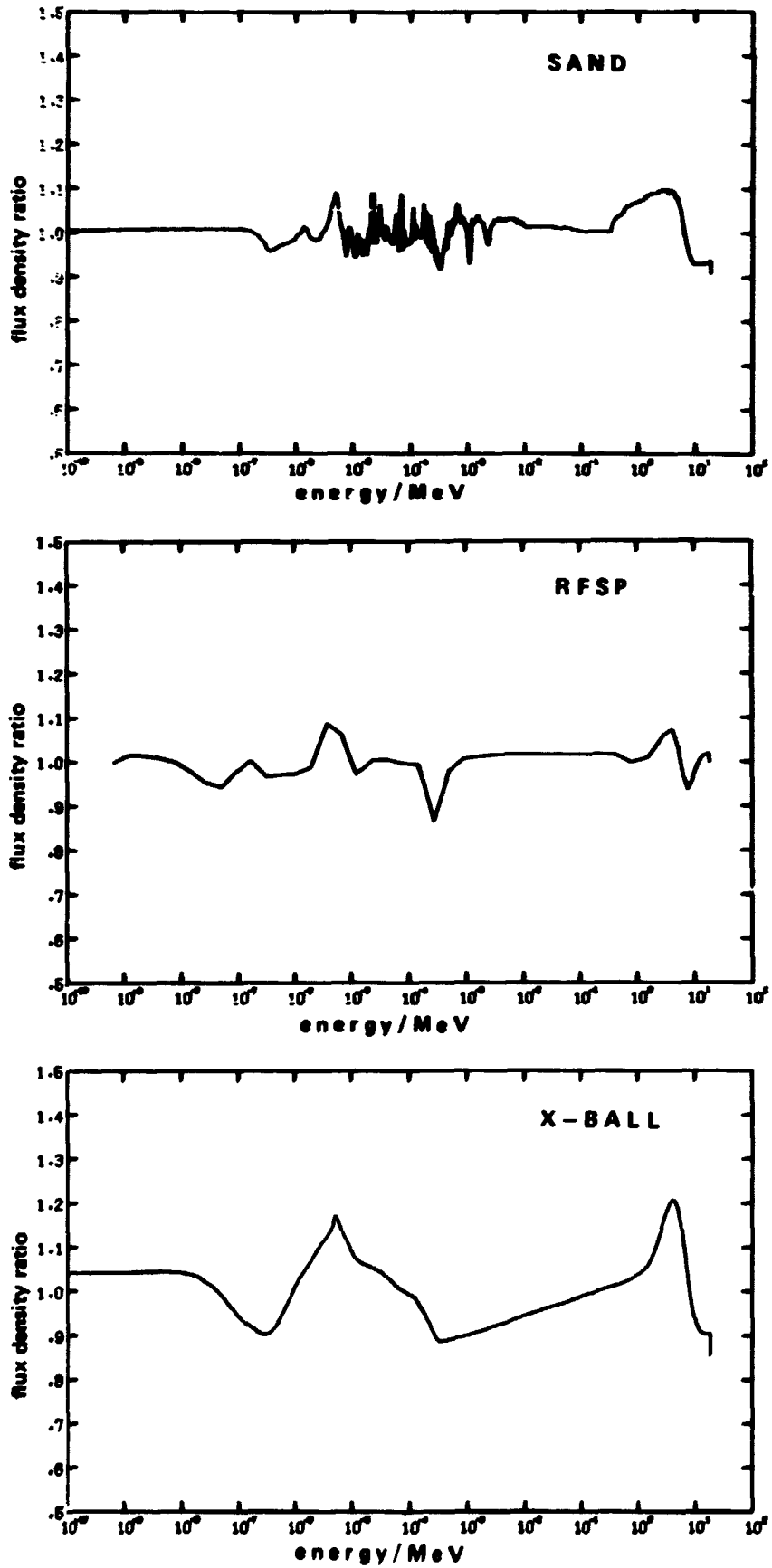


Fig. 6. Ratio of the input and output spectra for the three unfolding codes.
Results for the VC in the LFR.

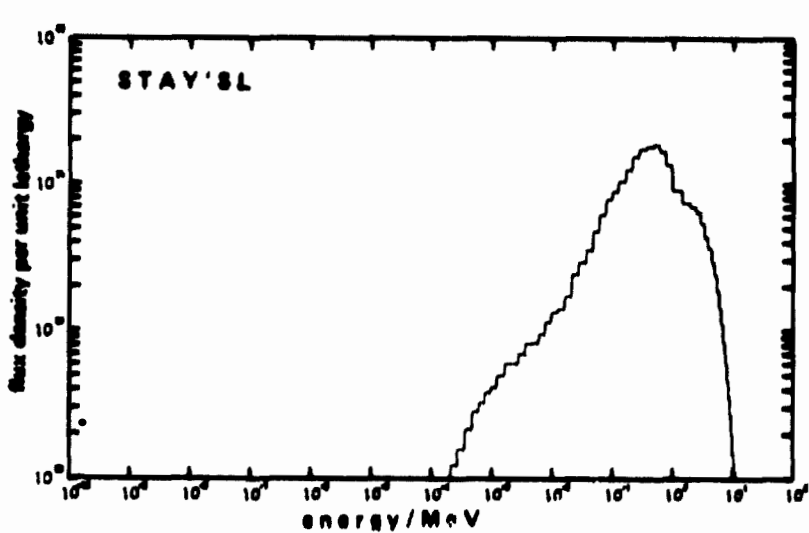
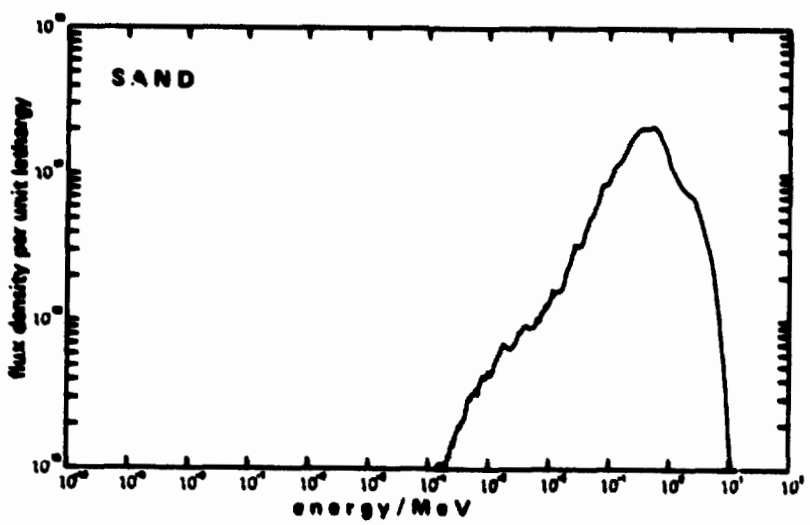
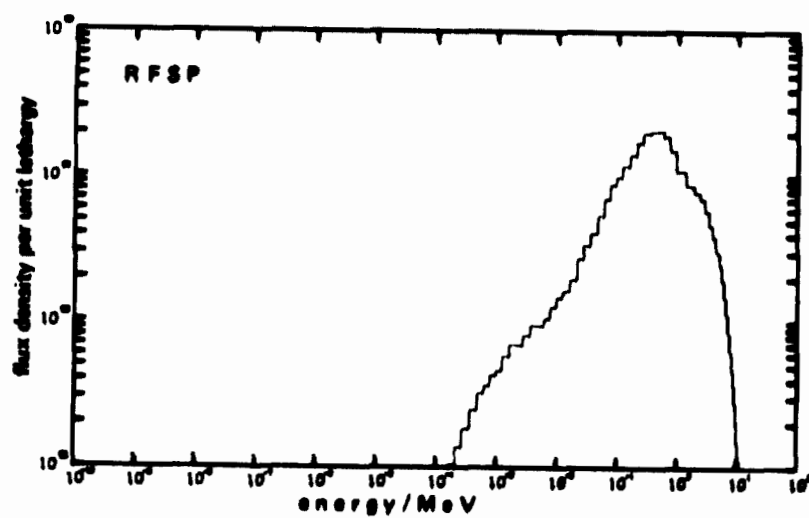
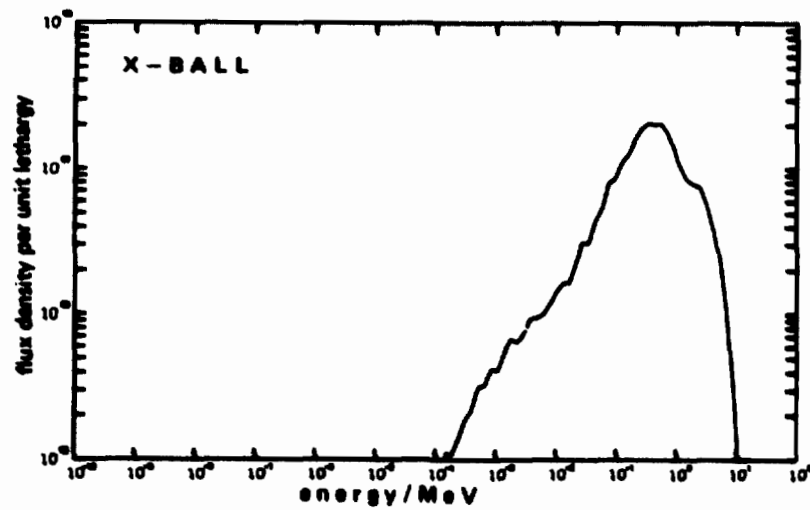


Fig. 7. Output spectra for CFRM[®] (with ARD ≈ 1.45).

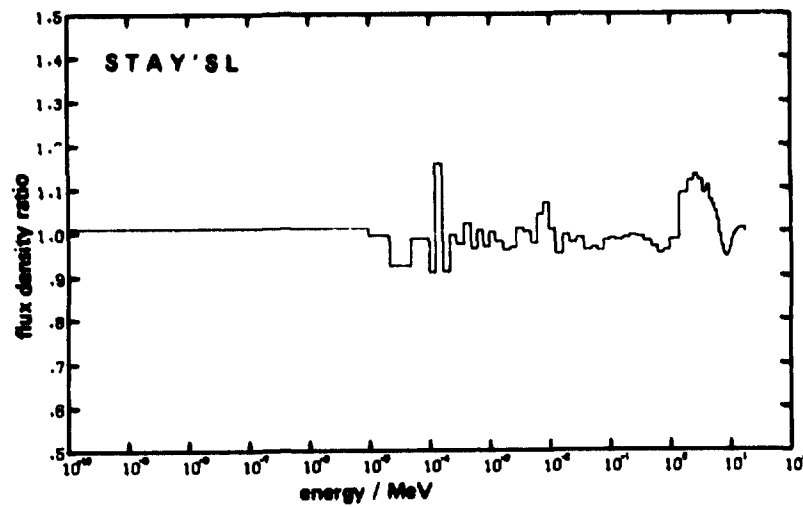
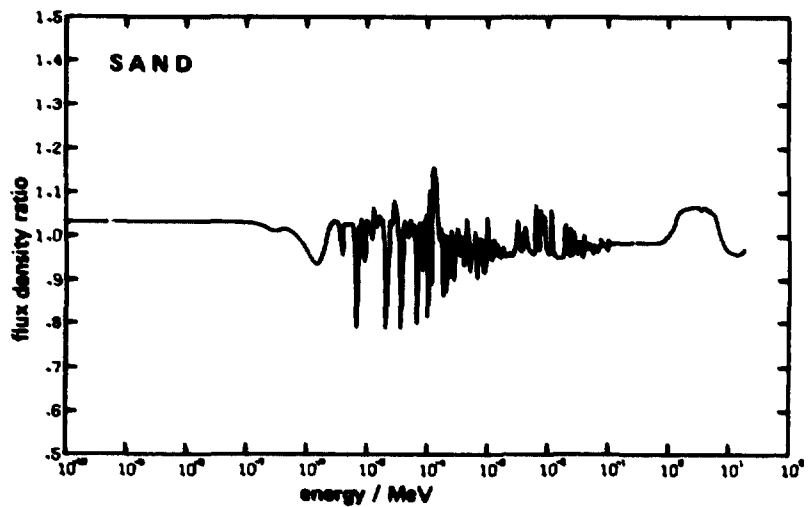
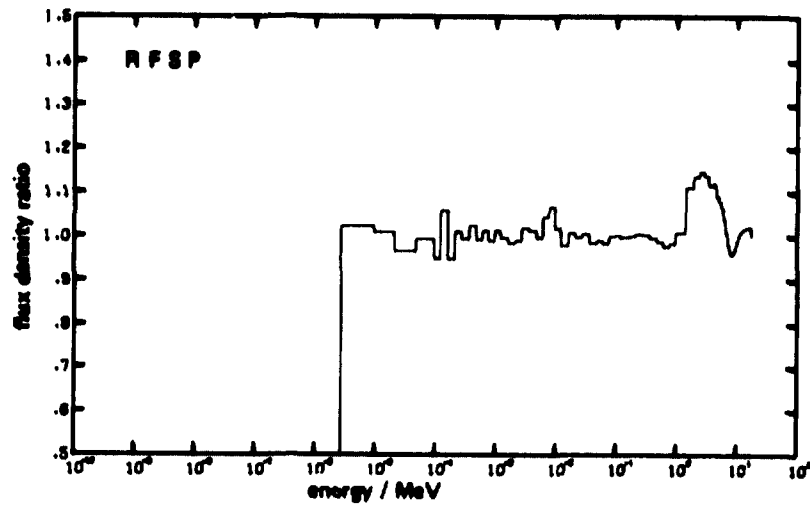
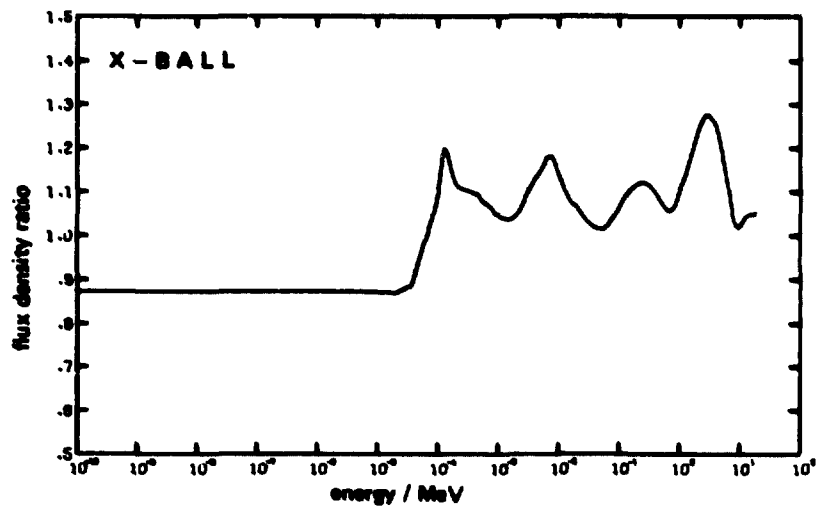


Fig. 8. Ratio of output flux densities and input flux densities for CFR² (with ARD \approx 1.45).

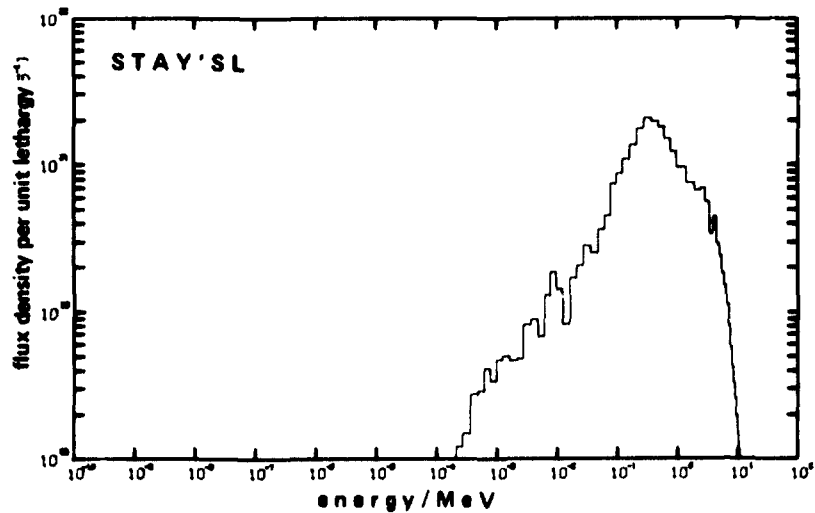
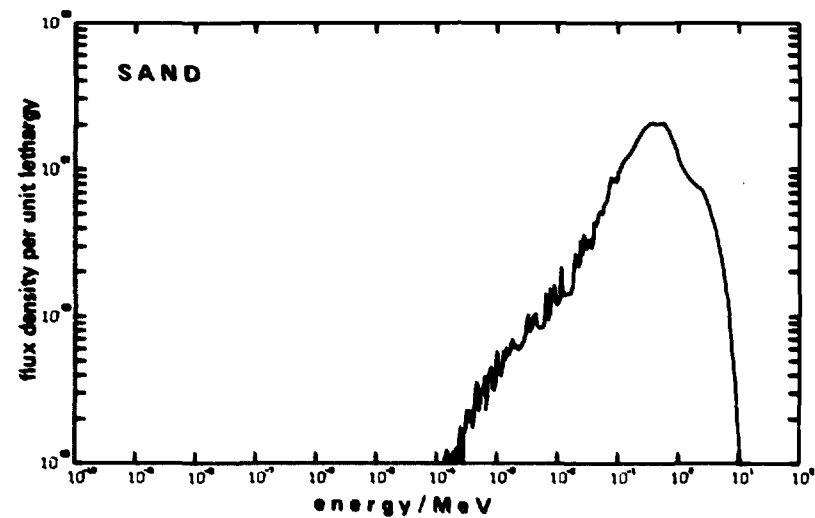
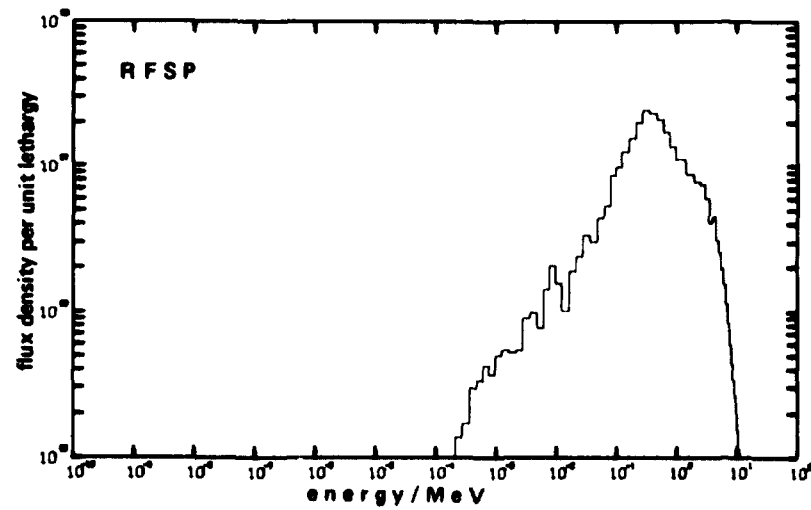
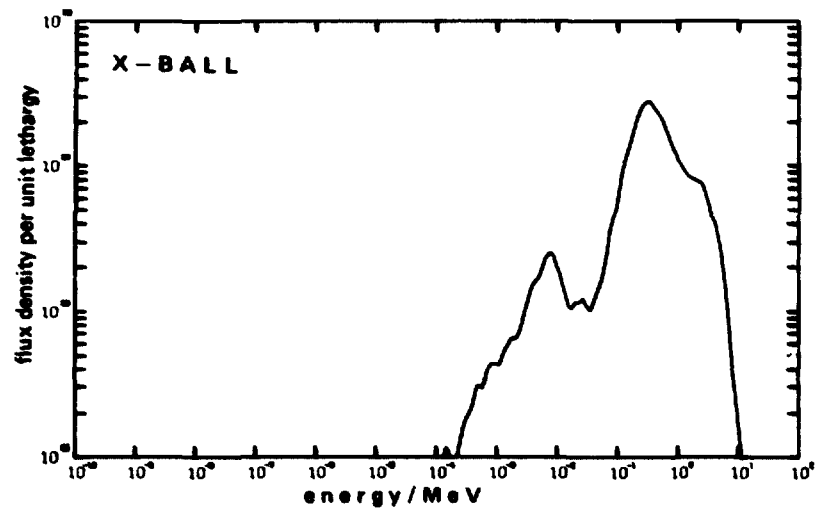


Fig. 9. Output spectra for CFRTF (with ARD \approx 1.00).

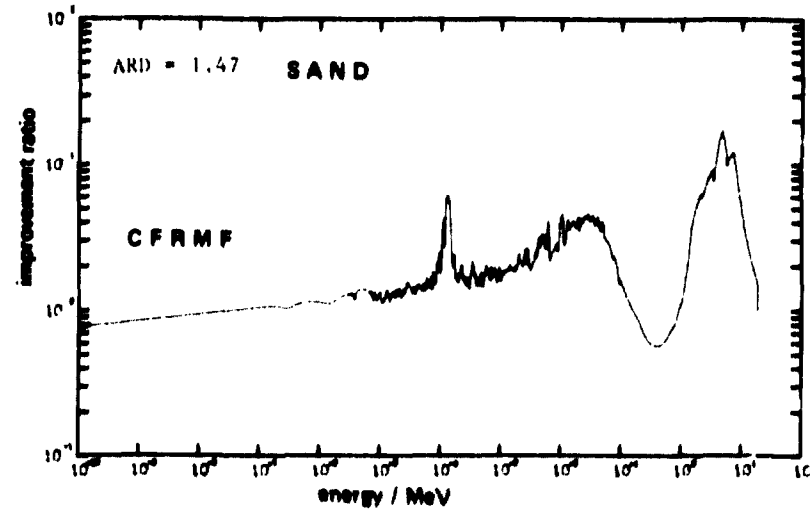
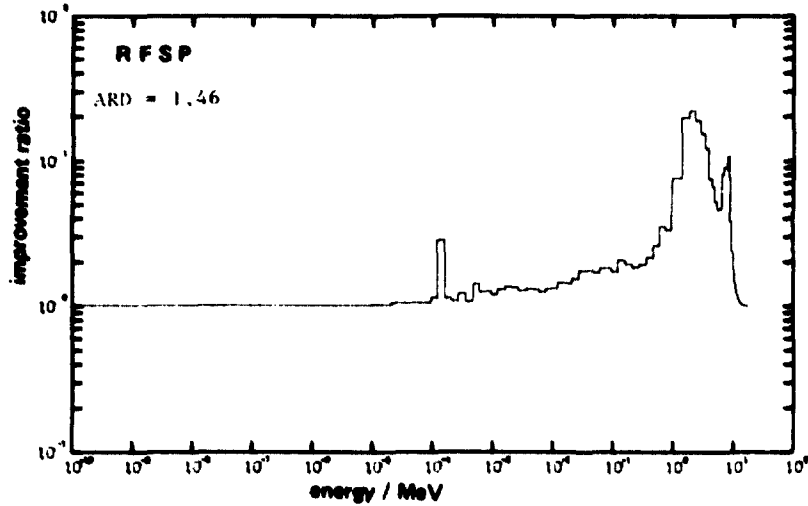
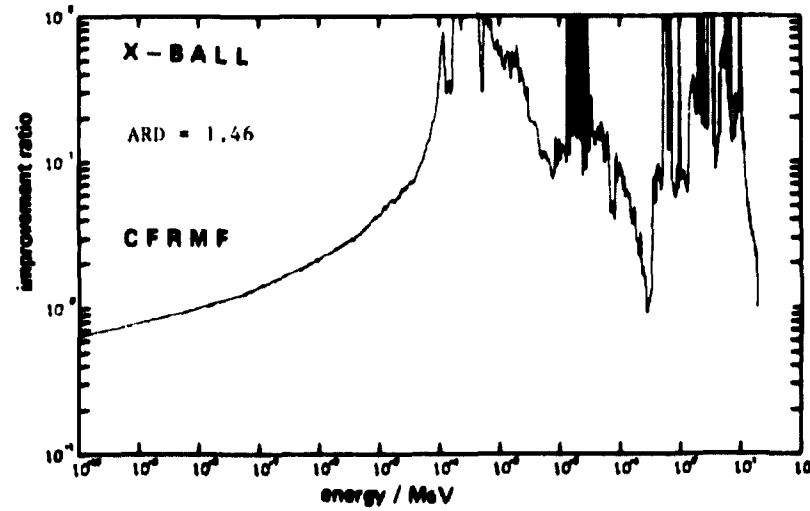
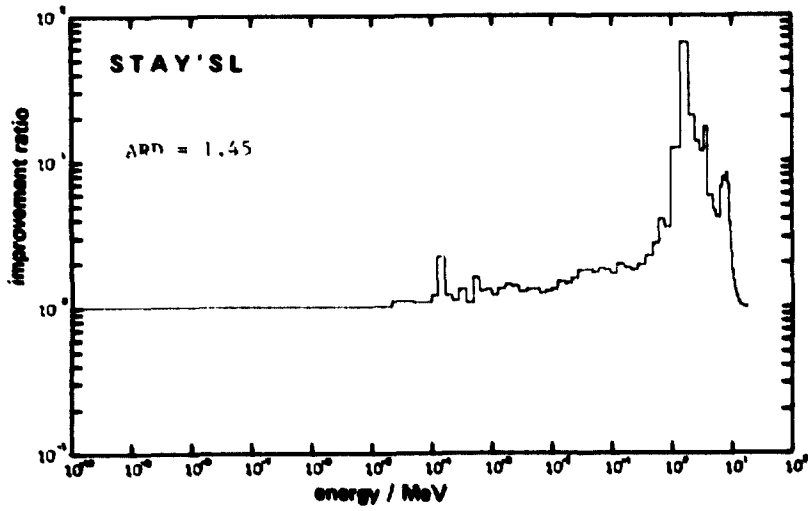


Fig. 10. The improvement ratio plots for CFRMF (with ARD = 1.45).

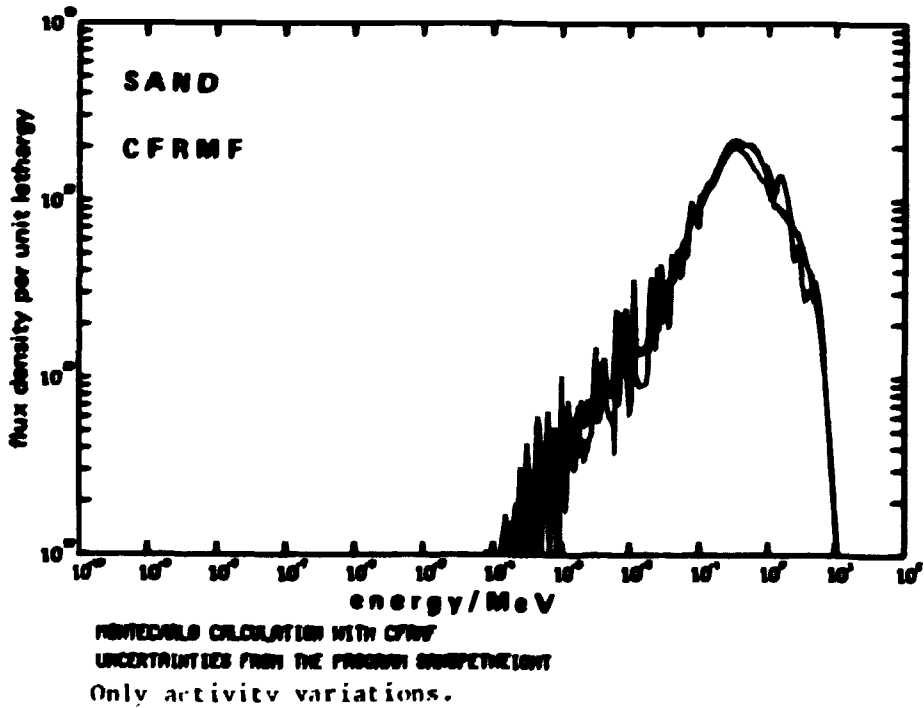
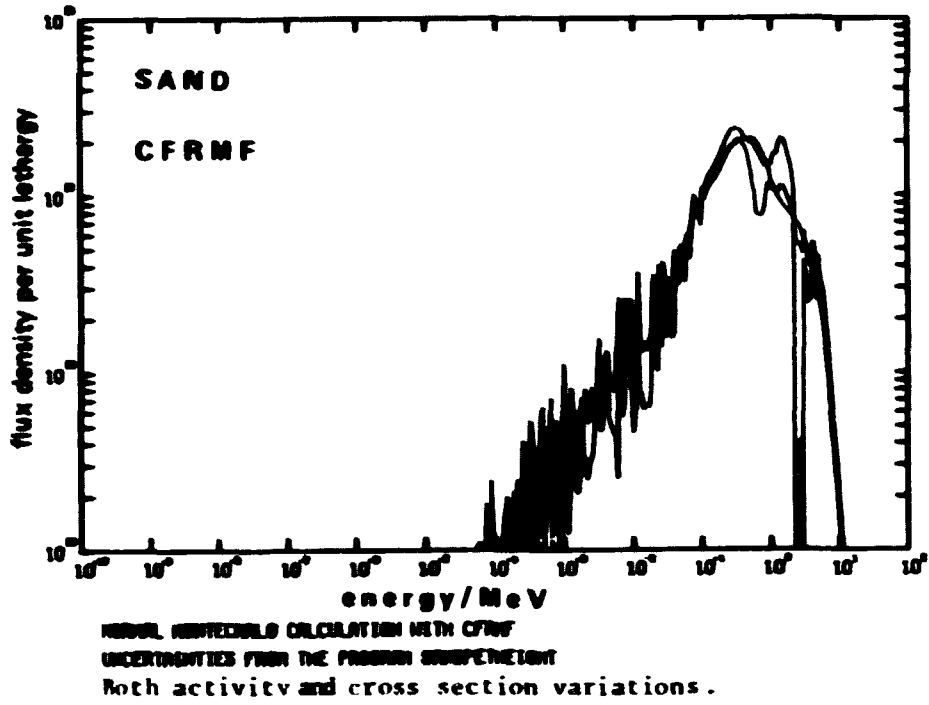


Fig. 11. The plots of the MonteCarlo results.