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Abstract

A new method for the neutron spectrum unfolding has been developed, based on the improvement of the generalized least squares method. The new method allows an iterative treatment of the problem and the number of the independent statistical variables of the solution is less than the number of the measured reaction rates. The capabilities of the method are demonstrated by a numerical experiment and by the solution of a real problem.

1. Introduction

The determination of the neutron spectrum from an integral experiment has an important and rising role in neutron dosimetry. Therefore, a lot of efforts have been made to check and improve the calculation methods.[1] Recently, the construction of fusion reactor blankets requires integral experiments to check the accuracy of the computational methods and the nuclear data used in the calculations.[2]

The problem of the neutron spectrum unfolding is the following: the activation rates a_i of n neutron reactions with different threshold energies are measured in a neutron field, and the neutron spectrum has to be determined from these data. The activation rates can be expressed as:

$$a_i = \int \phi(E)\sigma_i(E)dE \qquad (i=1..n) \qquad (1)$$

where a_i = reaction rate of the i-th neutron reaction
$\sigma_i(E)$ = excitation function of the i-th neutron reaction
$\phi(E)$ = unknown differential neutron flux

Several methods and computer codes have been developed for the solution of this problem.

If the neutron spectrum could be given in the form of an analytical function $f(E,a_1,...,a_m)$, containing $m \leq n$ parameters then

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the problem could be solved. Practically, this method is not used because in the real cases the neutron spectrum can not be written in the form of an analytical function. An interesting approach in this way is to approximate the neutron spectrum with spline functions [3].

The most frequently used solutions of the unfolding problem represent the neutron spectrum in numerical form i.e. the energy scale is divided into N energy groups and the differential flux is replaced by its average over these energy intervals. In the real cases the number of intervals is much more than the number of the activation rates (N>n); therefore, the system of equations can not be solved without some additional *a priori* information. Some unfolding codes such as SAND-II [4], SPECTRA [5], ITER [6] obtain their solution by introducing the additional information in the form of an *input or trial spectrum* and make an iterative refinement of this *input spectrum*. Naturally, the solution depends more or less on the input spectrum and if it is far from the real one the iteration procedure may stop at a local minimum. The main difficulty is that it isn't clear how the solution depends on the input spectrum.

A clearer solution has been proposed by F. G. Perey [7] based on the generalized least-squares method. The starting point of this solution is that the input spectrum is treated as if it would be taken from an earlier real measurement and it has a covariance matrix describing the variance and correlation of the input spectrum data. This input spectrum can be taken not only from experiment but also from neutron transport calculation. If a correct covariance information is available for the input spectrum, the generalized least-squares method gives a correct solution with correct covariance matrix (i.e. if the assumption of the model is valid the results will be correct.) This method has also some practical difficulties:

1. The activation method is preferred when other methods can not be used for the determination of the neutron spectrum, i.e. when there is no experimental input spectrum.
2. The calculation of the input neutron spectrum with a neutron transport code needs a lot of efforts and computation time. The calculations use several approximations and it is difficult to estimate their effect on the result.

3. Calculation of the covariance matrix of the input spectrum is much more difficult than the calculation of the spectrum itself. If the covariance matrix is incorrect then the result will be incorrect, too.

4. The statement that there is no need for iteration [7] is true only if the initial spectrum is close to the new solution. If the initial spectrum and its covariance matrix is correct from the statistical point of view, but the input spectrum is poorly determined then the solution should be iterated. After the first step, however, the input spectrum and the reaction rates become correlated; therefore, the equations derived in [7] must not be used for the iteration.

2. Solution without input spectrum.

Our aim was to solve the unfolding problem without *input spectrum*, because it is the most critical point of all numerical solutions. The principal reason why the unfolding codes need an input spectrum is the following: *The differential neutron flux on the energy grid consisting of N energy intervals are treated as N independent data i. e. the covariance matrix of the input spectrum has a rank of N.* If n activation rates are measured, only m≤n independent parameters can be determined. Suppose that the differential neutron flux can be given in the form of an analytical function with m parameters i. e. $\phi(E)=f(E,a_1,\ldots,a_m)$. After solving the unfolding problem we get a solution for the a_i parameters and the covariance matrix of these parameters N_α. This function can be tabulated as a number of points and we can construct from it a Φ vector as:

$$\Phi=\begin{bmatrix}\phi(E_1)\\ \vdots\\ \phi(E_i)\\ \vdots\\ \phi(E_N)\end{bmatrix} \qquad (i=1\ldots N) \qquad (2)$$

This consists of N independent data only if the covariance matrix of Φ is not given. But the covariance matrix of Φ can be calculated from the covariance matrix of the a_i parameters in the usual way:

$$N_\Phi=SN_\alpha S^+ \qquad (3)$$

where S is the sensitivity matrix whose ij-th element is $S_{ij}=\frac{\partial\phi_i}{\partial a_j}$ and (+) denotes matrix transpose. The rank of the matrix N_α is m

and therefore the rank of D_Φ is not higher than m as the matrix multiplication does not increase the rank of the matrix. The rank of the covariance matrix shows the number of free parameters used in the solution. Therefore, we are looking for a solution that is given in numerical form but its covariance matrix has a rank less than the number of the measurements (n). In this way the number of the free parameters are less than the number of the measurements and ,therefore, we do not need an *input spectrum* to overdetermine the unknown parameters. As our solution is given in numerical form, therefore, *a priori* analytical function is not necessary. We want to solve the unfolding problem in a way that the rank of the covariance matrix does not exceed the number of the measurements. The generalized least squares method does not increase the rank of the covariance matrix of the solution, but the usual derivation of this method assumes that the covariance matrix of the input spectrum is non-singular which is not true in our case. We can start from a first approximation whose rank is known and then we can transform our solution into a more detailed representation. We can also transform the covariance matrix of the first approximation into the new representation using Eq. 3. without increasing the rank of the covariance matrix.

The procedure that is called successive approximation may be the following:

1. Divide the energy range investigated into $m_o<n$ intervals and solve the unfolding problem approximately. In this case the the rank of the covariance matrix of the solution will be m_o. Therefore, the number of the unknown variables is less than that of the equations so the system of the equations can be solved. The solution will be Φ_1 and its covariance matrix D_1.
2. Transform this solution into a more detailed energy grid with a (linear) interpolation:

   $$\Phi_{2o}=S_1\Phi_1 \qquad D_{2o}=S_1 D_1 S_1^+ \qquad (4a,b)$$

   where Φ_{2o} is the new initial approximation of the differential neutron flux and D_{2o} is its covariance matrix. The rank of D_{2o} does not increase because matrix multiplication is used.
3. Solve the unfolding problem with this new approximation.
4. Repeat step 2 and 3 until the requested density of the energy grid is reached.

To solve the unfolding problem in this way, a modified version of the generalized least-squares method is needed because the

covariance matrix of the solution is singular and an iterative solution of the problem is required. The iterative solution means the Φ_{io} and the original data set (a_i) are correlated because Φ_{io} is determined from the measured data.

3. Iterative solution of the generalized method of the least squares.

Muir [8] derived the generalized method of least squares on the basis of the minimum variance approach. This derivation allows the nonlinearity of the problem, correlation between measured data and calculated parameters, non-normal distribution of the statistical variables and non-singularity of the covariance matrix of the parameter vector. It is assumed that there is an initial set of parameters p_i (denoted by the vector P) that one wishes to improve by taking into account new measurement of certain relevant physical quantities. Let the result of the new measurement the vector D_o while D(P) are the same physical quantities calculated from the parameters p_i; then the information content of the new measurement can be represented in terms of the discrepancy vector,

$$X=D_o-D \qquad (5)$$

The best adjustment of any vector Z that depends on these physical quantities can be calculated as follows:

$$Z'=Z-\mathrm{cov}(Z,X)\mathbb{N}_x^{-1}X \qquad (6a)$$

$$\mathbb{N}_{Z'}=\mathbb{N}_Z-\mathrm{cov}(Z,X)\mathbb{N}_x^{-1}\mathrm{cov}(Z,X)^+ \qquad (6b)$$

where Z' is the improved estimate of the Z vector and $\mathbb{N}_x$, $\mathbb{N}_z$, $\mathbb{N}_{z'}$ are the covariance matrices of X,Z,Z', respectively. The cov(Z,X) denotes a rectangular matrix whose ij-th element is the pre-adjusted covariance $\mathrm{cov}(z_i,x_j)$.

As correlation between the vectors is allowed we can apply these equations to the iterative solution of the problem. Consider a non-linear case which is linearized near the P_{10} point. In this case the fit function is

$$D'=D_1+\mathbb{G}(P_{10})(P'-P_{10}) \qquad (7)$$

where $\mathbb{G}(P_{10})$ is the sensitivity matrix with elements $G_{ij}=\dfrac{\partial D_i}{\partial P_j}$ and D_1 is the calculated value of D in the P_{10} point. If P_{10} and D_o are independent then the improved P_1 vector is the following:

$$P_1=P_{10}-\mathrm{cov}(P_{10},D_o-D_1)\left[\mathrm{cov}(D_o-D_1,D_o-D_1)\right]^{-1}(D_o-D_1).$$

However,

$$\mathrm{cov}(P_{10}, D_0 - D_1) = \mathrm{cov}(P_{10}, D_0) - \mathrm{cov}(P_{10}, D_1) = -\mathrm{cov}(P_{10}, G_1 P_{10}) = -N_{P_{10}} G_1^+$$

since P_{10} and D_0 are independent, and

$$N_{X_1} = \mathrm{cov}(D_0 - D_1, D_0 - D_1) = \mathrm{cov}(D_0, D_0) + \mathrm{cov}(D_1, D_1) - \mathrm{cov}(D_0, D_1) - \mathrm{cov}(D_1, D_0)$$

$$\mathrm{cov}(D_0 - D_1, D_0 - D_1) = M + \mathrm{cov}(GP_{10}, GP_{10}) = M + G_1 N_{P_{10}} G_1^+$$

since D_0 and D_1 are independent. Then the final result for P_1 is

$$P_1 = P_{10} + N_{P_{10}} G_1^+ \left[M + G_1 N_{P_{10}} G_1^+ \right]^{-1} (D_0 - D_1) \qquad (8a)$$

and its covariance matrix is

$$N_{P_1} = N_{P_{10}} - N_{P_{10}} G_1^+ \left[M + G_1 N_{P_{10}} G_1^+ \right]^{-1} G_1 N_{P_{10}} \qquad (8b)$$

These expressions for the improved estimation are exactly the same as obtained in the usual way of the generalized least squares derivation. But now P_1 and D_0 are not independent and their covariance L_1 can be calculated as:

$$L_1 = \mathrm{cov}(P_1, D_0) = \mathrm{cov}(P_{10} + N_{P_{10}} G_1^+ \left[M + G_1 N_{P_{10}} G_1^+ \right]^{-1} (D_0 - D_1), D_0)$$

$$L_1 = N_{P_{10}} G_1^+ \left[M + G_1 N_{P_{10}} G_1^+ \right]^{-1} M. \qquad (9)$$

Our aim is to transform the solution to another energy grid with a linear transformation and then to improve the solution. Denote this transformation by S_i in the i-th step; then the new initial vector and its covariance matrix will be the following:

$$P_{i0} = S_{i-1} P_{i-1} \quad \text{and} \quad N_{P_{i0}} = S_{i-1} N_{P_{i-1}} S_{i-1}^+ \qquad (10a,b)$$

Suppose that we have calculated the (i-1)-th step and now the i-th step is being performed. Introduce the K_i matrix by the following definition: $K_i = -\mathrm{cov}(P_{i0}, D_0 - D_i)$. Then

$$K_i = \mathrm{cov}(P_{i0}, D_i) - \mathrm{cov}(P_{i0}, D_0) = N_{P_{i0}} G_i^+ - \mathrm{cov}(S_{i-1} P_{i-1}, D_0)$$

$$K_i = N_{P_{i0}} G_i^+ - S_{i-1} \mathrm{cov}(P_{i-1}, D_0) = N_{P_{i0}} G_i^+ - S_{i-1} L_{i-1}$$

Let $B_i = \mathrm{cov}(D_i, D_0)$, then it can be expressed as

$$B_i = \mathrm{cov}(D_i, D_0) = \mathrm{cov}(G_i P_{i0}, D_0) = \mathrm{cov}(G_i S_{i-1} P_{i-1}, D_0) = G_i S_{i-1} L_{i-1}$$

Using these abbreviations one can get for N_{X_i}

$$N_{X_i} = M + G_i N_{P_{io}} G_i^+ - B_i - B_i^+$$

So both K_i and N_{X_i} can be taken from the previously calculated matrices and now the new sensitivity matrix, the new improved vector, as well as its covariance matrix can be calculated.

$$P_i = P_{io} + K_i N_{X_i}^{-1} (D_o - D_i)$$

$$N_{P_i} = N_{P_{io}} - K_i N_{X_i}^{-1} K_i^+$$

The new L_i can be determined in the following way:

$$L_i = \mathrm{cov}(P_i, D_o) = \mathrm{cov}(P_{io} + K_i N_{X_i}^{-1} (D_o - D_i), D_o)$$

$$L_i = S_{i-1} L_{i-1} + K_i N_{X_i}^{-1} \mathrm{cov}(D_o - D_i, D_o) = S_{i-1} L_{i-1} + K_i N_{X_i}^{-1} (M - B_i)$$

Summarizing, the equations of the iterative solution of the generalized least squares method are

$$P_i = P_{io} + K_i N_{X_i}^{-1} (D_o - D_i) \qquad (11a)$$

$$N_{P_i} = N_{P_{io}} - K_i N_{X_i}^{-1} K_i^+ \qquad (11b)$$

$$L_i = S_{i-1} L_{i-1} + K_i N_{X_i}^{-1} (M - B_i) \qquad (11c)$$

where

$$B_i = G_i S_{i-1} L_{i-1} \qquad (11d)$$

$$N_{X_i} = M + G_i N_{P_{io}} G_i^+ - B_i - B_i^+ \qquad (11e)$$

$$K_i = N_{P_{io}} G_i^+ - S_{i-1} L_{i-1} \qquad (11f)$$

$$P_{io} = S_{i-1} P_{i-1} \qquad N_{P_{io}} = S_{i-1} N_{P_{i-1}} S_{i-1}^+ \qquad (11g,h)$$

with

$$L_o = 0 \qquad S_o = I$$

initial matrices.

This solution can be applied for any problem that needs the iterative solution of the least-squares method. Usually, the transformation between the iterative steps are not used. In these cases the substitution $S_i = I$ is needed.

4. Solution of the unfolding problem by successive approximation

Assume that we know the values of the excitation functions at N points and their covariance matrices for n reactions. Usually N>n because the good representation of the excitation function need a fine energy grid structure. Let us divide the energy range investigated $[E_o, E_{max}]$, where $\phi(E)>0$ and there is at least one $\sigma_i(E)>0$, into m<N energy intervals. The reaction rates can be written into the following form:

$$a_i = \sum_{j=1}^{m} \int_{E_j}^{E_{j+1}} \phi(E)\sigma_i(E)dE \qquad (i=1..n) \qquad (12)$$

where $E_1=E_o$ and $E_{m+1}=E_{max}$. Since $\phi(E)>0$, the reaction rates can be transformed into the following form:

$$a_i = \sum_{j=1}^{m} \int_{E_j}^{E_{j+1}} \phi(E)dE \; \frac{\int_{E_j}^{E_{j+1}} \phi(E)\sigma_i(E)dE}{\int_{E_j}^{E_{j+1}} \phi(E)dE} \qquad (i=1..n). \qquad (13)$$

Introducing the notations:

$$\langle\phi_j\rangle_E = \frac{1}{E_{j+1}-E_j} \int_{E_j}^{E_{j+1}} \phi(E)dE \qquad (14a)$$

$$\langle\sigma_{ij}\rangle_{E,\phi} = \frac{\int_{E_j}^{E_{j+1}} \phi(E)\sigma_i(E)dE}{\int_{E_j}^{E_{j+1}} \phi(E)dE} \qquad (14b)$$

and

$$\langle\sigma_{ij}\rangle_E = \frac{1}{E_{j+1}-E_j} \int_{E_j}^{E_{j+1}} \sigma_i(E)dE, \qquad (14c)$$

the reaction rates become

$$a_i = \sum_{j=1}^{m} \langle\phi_j\rangle_E \langle\sigma_{ij}\rangle_{\phi,E} (E_{j+1}-E_j) \qquad (i=1....n) \qquad (15)$$

The $\langle\sigma_{ij}\rangle_{\phi,E}$ values are unknown; therefore, we have to estimate them. The simplest way to do this is to substitute $\langle\sigma_{ij}\rangle_E$ for $\langle\sigma_{ij}\rangle_{\phi,E}$.

$$a_i \cong \sum_{j=1}^{m} \langle\phi_j\rangle_E \langle\sigma_{ij}\rangle_E (E_{j+1}-E_j) \qquad (i=1.....n) \qquad (16)$$

Since we get $\sigma_i(E)$ from experiments, we never know their exact values, only estimate and their variances. Therefore, we can use the sign of equality instead of $\cong$ if we can estimate the errors of using $\langle\sigma_{ij}\rangle_E$ instead of $\langle\sigma_{ij}\rangle_{\phi,E}$. From physical reasons $\phi(E)>0$ and $\sigma_i(E)\geq 0$. Therefore,

$$\min_{[E_j,E_{j+1}]} \langle\sigma_i(E)\rangle \leq \langle\sigma_{ij}\rangle_{\phi,E} \leq \max_{[E_j,E_{j+1}]} \langle\sigma_i(E)\rangle \qquad (17a)$$

$$\min_{[E_j,E_{j+1}]} \langle\sigma_i(E)\rangle \leq \langle\sigma_{ij}\rangle_E \leq \max_{[E_j,E_{j+1}]} \langle\sigma_i(E)\rangle \qquad (17b)$$

where min( ) and max( ) denote the minimum and maximum values of the argument in the given energy interval, respectively. Both $\langle\sigma_{ij}\rangle_{\phi,E}$ and $\langle\sigma_{ij}\rangle_E$ are between the same limits and their difference can be small if the $\sigma_i(E)$ does not change too much over the energy interval $[E_j,E_{j+1}]$. On the other hand, it can be large if the excitation function of the reaction decreases or increases sharply in this energy interval. Therefore, it seems a reasonable estimation for the variance of the deviation of $\langle\sigma_{ij}\rangle_{\phi,E}-\langle\sigma_{ij}\rangle_E$:

$$\frac{\sigma_i^{O}{}_{jj}}{(E_{j+1}-E_j)^2} = \mathrm{var}(\langle\sigma_{ij}\rangle_{\phi,E}-\langle\sigma_{ij}\rangle_E) \approx \frac{1}{E_{j+1}-E_j}\int_{E_j}^{E_{j+1}} (\sigma_i(E)-\langle\sigma_{ij}\rangle_E)^2 dE \qquad (18)$$

Let us introduce a diagonal matrix Φ_i with elements given in (18). Denote the values $\langle\sigma_{ij}\rangle_E(E_{j+1}-E_j)$ by Σ_{ij}, its correspondent values in the original fine grid structure by Σ^N_{ij}, and to simplify the notation we introduce the cross section vectors $\bar{\Sigma}_i$ and $\bar{\Sigma}^N_i$. As we know the original and the new energy grid, we can generate a $\mathbb{C}$ matrix which transforms the original $\bar{\Sigma}^N_i$ vector to the new one. With this transformation we can get the new covariance matrix, too, taking into account the correction introduced above.

$$\bar{\Sigma}_i = \mathbb{C}\bar{\Sigma}^N_i \qquad \mathbb{N}_i = \mathbb{C}\mathbb{N}^N_i\mathbb{C}^+ + \Phi_i \qquad (19a,b)$$

Using this notation and constructing a Φ vector from $\langle\phi_j\rangle$ the reaction rates can be written as

$$a_i = \bar{\Sigma}^+_i \Phi \qquad (20)$$

In solving this system of equation we have to take into account

that the average cross sections also have errors. This can be done [7] by introducing the parameter vector P and its covariance matrix

$$P=\begin{pmatrix}\Phi\\ \Sigma_1\\ .\\ \Sigma_m\end{pmatrix} \quad \text{and} \quad \mathbb{N}_P=\begin{pmatrix}\mathbb{N}_\Phi & 0 & . & 0\\ 0 & \mathbb{N}_1 & & 0\\ . & & . & .\\ 0 & 0 & & \mathbb{N}_m\end{pmatrix}. \qquad (21a,b)$$

Here the excitation functions of the different reactions are considered to be independent; this, however, is not necessary. In this case a_i is a bilinear product of some elements of P; therefore, our model is nonlinear. To get the sensitivity matrix we must linearize the model by performing an expansion about the estimated expectation value of Φ and Σ, and we get

$$a_i'=\bar{\Sigma}_i^+\Phi+\Phi^+(\bar{\Sigma}_i'-\bar{\Sigma}_i)+\bar{\Sigma}_i^+(\Phi'-\Phi)+(\bar{\Sigma}_i'-\bar{\Sigma}_i)^+(\Phi'-\Phi). \qquad (22)$$

We have to drop the last term only to become the model linear, therefore, our model is very near to a linear one. Comparing this with the expression

$$D'=D_1+\mathbb{G}(P_{10})(P'-P_{10}) \qquad (23)$$

we get

$$\mathbb{G}=\begin{pmatrix}\bar{\Sigma}_1^+ & \Phi^+ & 0 & 0 & \dots\\ \bar{\Sigma}_2^+ & 0 & \Phi^+ & 0 & \dots\\ \bar{\Sigma}_3^+ & 0 & 0 & \Phi^+ & \dots\\ . & . & . & . & \\ . & . & . & . & \end{pmatrix}. \qquad (24)$$

Since our problem is nonlinear we need an initial vector P_{10} to start the iteration procedure. We choose an energy grid where the number of the energy intervals, m_o, is less than n, the number of the measured reaction rates. This m_o will determine the free parameters of the neutron spectrum during the evaluation. The vectors $\bar{\Sigma}_i$ are known, so we have to create only the vector Φ_o. Considering eq. 20. with constant vectors $\bar{\Sigma}_i^+$ we have $m_o<n$ unknown variable for a system of equation consisting of n equations. Therefore, this can be solved by the usual linear least squares procedure. Introducing the matrix $\mathbb{G}_o$ as

$$\mathbb{G}_o=\begin{pmatrix}\bar{\Sigma}_i^+\\ \vdots\\ \bar{\Sigma}_i^+\end{pmatrix} \qquad (25)$$

and the vector D_o containing the measured reaction rates and $\mathbb{M}$ for its covariance matrix, then Φ_o can be calculated as

$$\Phi_o=(\mathbb{G}_o^+\mathbb{M}^{-1}\mathbb{G}_o)^{-1}\mathbb{G}_o^+\mathbb{M}^{-1}\mathbb{D}_o \qquad (26)$$

We could calculate the covariance matrix of Φ_o but in this case we do not take into account the errors of $\bar{\Sigma}_i^+$ which is very important because we approximate the original equations. Therefore, we consider this Φ_o as the starting point of the iteration without real information content. So we generate its covariance matrix in the following form: the diagonal elements contain very large values (for example 100% standard deviation) and the other elements are set to zero. This is the reason why we may suppose that this initial vector has no correlation with D_o. Putting this Φ_o into P_{1o} and its covariance matrix into $N_{P_{1o}}$ eq. (20) can be solved with the generalized least squares method and we get a real estimation for the covariance matrix. We have included the $\bar{\Sigma}_i$ vector into P in order to propagate their uncertainties to the solution. The cross sections are assumed to be only "formally adjustable" during the calculation. This takes into account that our model (i.e. eq. 20) is inexact. After obtaining the solution of the first step, we can expand the solution of Φ into a new, finer energy grid with an interpolation procedure. The new $\bar{\Sigma}_i$ vectors are generated in every step from the original $\bar{\Sigma}_i^N$ vectors; therefore, our model will be more and more exact. Using the previously introduced iterative solution of the generalized least squares method we can treat correctly the error propagation during the process. This iterative procedure is to be continued, at least, until the original energy grid is achieved. Since neither the linear interpolation nor the generalized least squares method does increase the rank of the covariance matrix, the rank of N_Φ will not be higher than m_o, i.e. the number of the free parameters in Φ is not higher than m_o.

5. Test of the successive approximation method.

A computer program (SULSA), written in FORTRAN, was developed for an IBM PC/XT compatible computer to solve the unfolding problem by the successive approximation method. The present version of the code uses diagonal cross section covariance matrices and an equidistant grid for $\bar{\Sigma}_i^N$. For testing purposes an artificial spectrum has been generated, which is the sum of an exponential and a Gauss type functions. The activation rates for 10 neutron reactions were calculated using this artificial spectrum (exact data) and 1% standard deviations were associated to them.

Table I. Input reaction rates in 10^{-19}/s, difference of the input and the calculated ones in percentage, and the global parameters of the unfolding.

	Exact data		Random-1		Random-2	
Reaction	Reaction rate	Dif. [%]	Reaction rate	Dif. [%]	Reaction rate	Dif. [%]
$Ni^{58}(n,p)Co^{58}$	3042.0	-0.42	3020.0	-5.07	2969.0	0.62
$Fe^{54}(n,p)Mn^{54}$	2058.0	-0.41	2636.0	2.62	2274.0	-4.42
$Al^{27}(n,\alpha)Na^{24}$	359.0	-0.39	356.0	-0.98	335.0	-5.57
$Co^{59}(n,2n)Co^{58}$	354.0	0.13	351.0	0.29	356.0	-1.19
$Au^{197}(n,2n)Au^{196}$	4284.0	-0.10	4274.0	-0.20	4033.0	-2.09
$Cu^{56}(n,p)Ni^{56}$	64.3	0.25	67.6	4.08	63.5	-0.05
$Ti^{48}(n,p)Sc^{48}$	139.0	0.01	135.0	-2.56	149.0	7.86
$In^{115}(n,n')In^{115m}$	1939.0	-0.07	1986.0	0.46	1958.0	0.30
$Y^{89}(n,2n)Y^{88}$	197.0	-0.61	189.0	-3.87	206.0	1.71
$Zr^{90}(n,2n)Zr^{89}$	104.0	-0.77	101.0	3.00	99.4	-7.50
χ_a^2	0.156		0.324		0.712	
χ_ϕ^2	1.13		0.943		1.31	

Two other data sets (random-1, random-2) for the reaction rates were generated by randomly altering the exact data with 5% standard deviation. Using these data sets three neutron spectra were evaluated. Two global parameters were calculated for every solution to test their acceptability:

$$\chi_a^2=\frac{1}{n}(\mathbb{D}_o-\mathbb{D})^T\mathbb{M}^{-1}(\mathbb{D}_o-\mathbb{D}) \qquad (27)$$

$$\chi_\Phi^2=\frac{1}{N}\sum_{i=1}^{N}\frac{(\phi_i-\phi_{io})^2}{N_{\phi_{ii}}} \qquad (28)$$

where $\mathbb{D}_o$, $\mathbb{D}$ are the vectors of the input and output activation rates, $\mathbb{M}$ is the covariance matrix of $\mathbb{D}_o$, while ϕ_{io}, ϕ_i and $N_{\phi_{ii}}$ are the original artificial, the calculated differential neutron flux and the diagonal element of its covariance matrix, respectively. The input data and the results of the calculation are summarized in Table I. and Figures 1.÷3. In the calculation the number of the reaction rates was 10 and m_o i.e. initial number of the intervals was chosen to 8. The value of m_o was increased by 50% in every

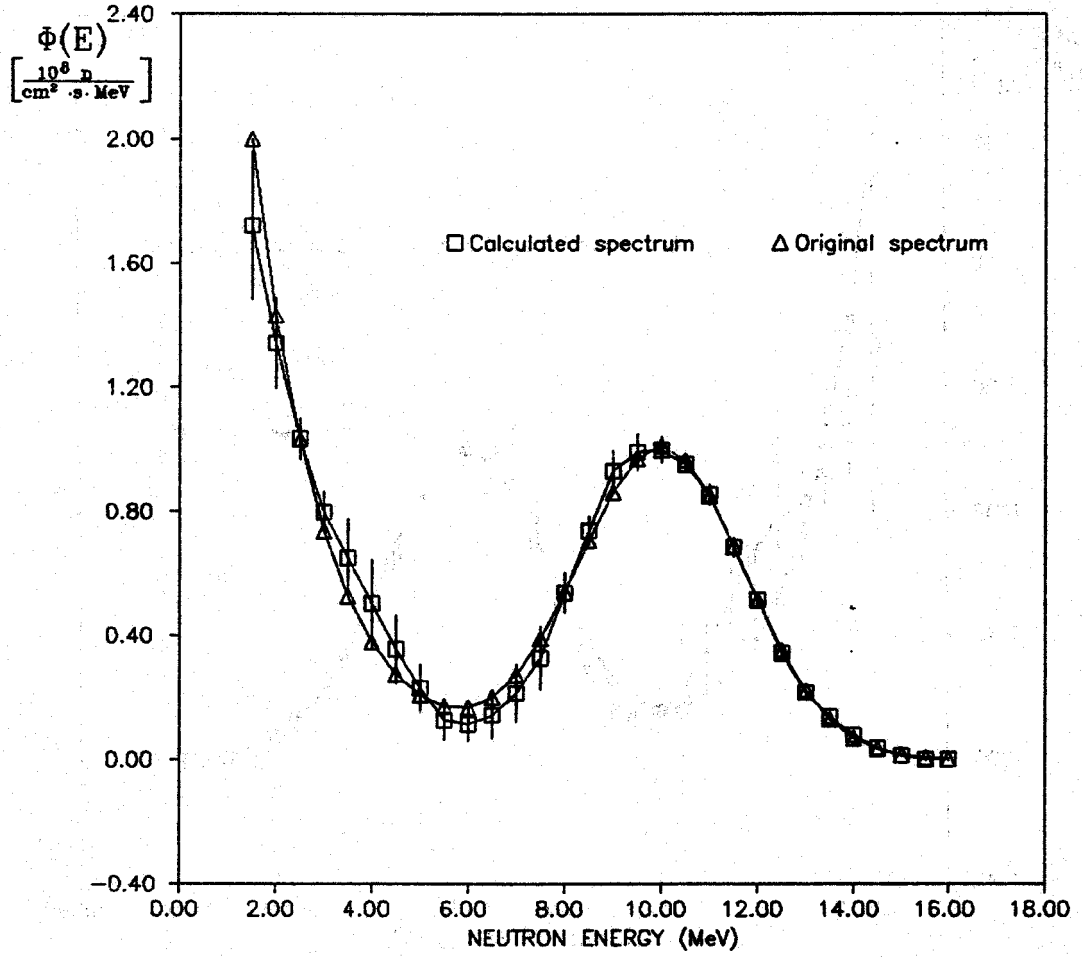

Figure 1. Comparison of the original and calculated spectra using the exact data set for the reaction rates.

iteration step until the final grid of 30 energy intervals was reached. Both χ_a and χ_Φ shows good solution both for the calculated reaction rates and for the differential neutron flux. In the case of the exact data the χ_a value is low arising from the overestimation of the error of the reaction rates. Figures 1.÷3. show the original artificial spectrum and the calculated ones for comparison. It can be seen that in all three cases the original function is very well approximated in the high energy range where the errors are small, while the low energy range shows larger deviations and stronger sensitivity for the values of the reaction rates. To see the goodness of the error estimation, Figure 4. shows the quantity $(\phi_i-\phi_{io})/\sqrt{N_{ii}}$ as function of the energy. It can be seen that the error estimation is correct, independently of the value of the error which is changing from a few per cent to more than hundred per cent.

Beside this artificial spectrum the program was tested with real measured data. Figure 5. shows the result of such a calculation

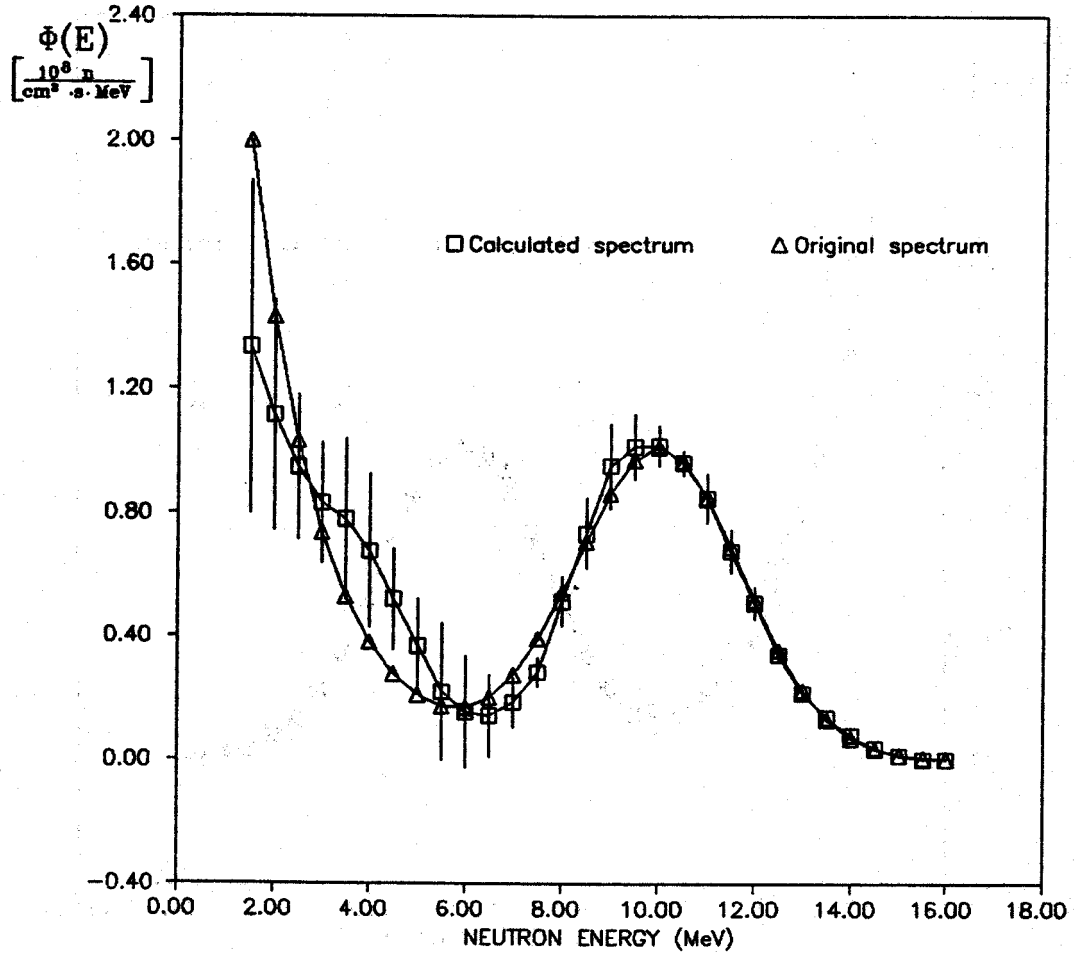

Figure 2. Comparison of the original and calculated spectra using the random-1 data set for the reaction rates.

where a differential neutron spectrum from the Be+d reaction at 17.5 MeV deuteron energy was calculated from our earlier measurements [8]. For comparison, the result of the SAND-II calculation is also shown. The shape of the solutions is very similar. There are only two regions where the deviations are significant: from 4 to 6 MeV and from 13 to 16 MeV. In the first interval the deviation is less than twice the calculated error, but in the second region the new solution seems to be more realistic because there is no physical reason for the long, almost constant differential neutron flux. Unfortunately, we do not know the real spectrum; therefore, we can not decide which is the better solution. The aim of the present work is to demonstrate that the model is working in a real case, too.

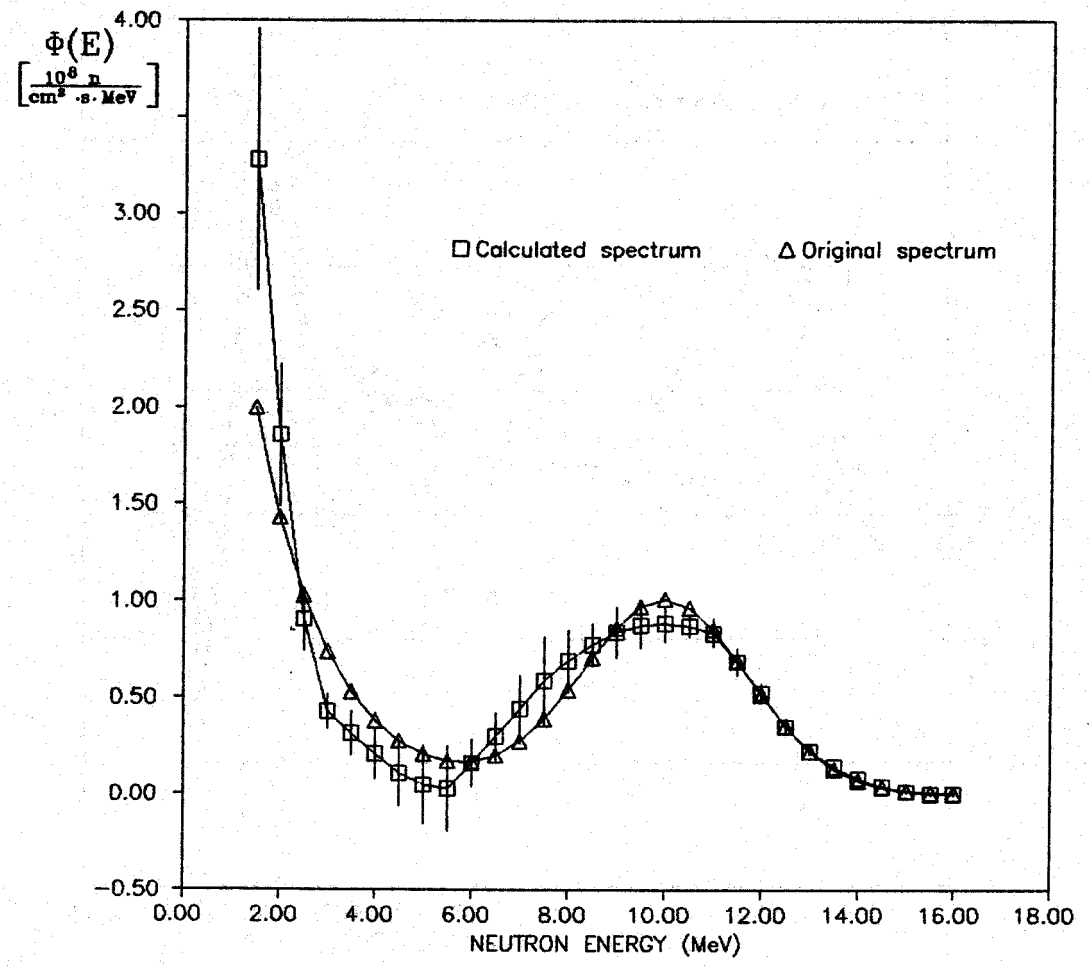

Figure 3. Comparison of the original and calculated spectra using the random-2 data set for the reaction rates.

6. Summary

The successive approximation method which is based on the iterative solution of the generalized least squares method and keeps the number of the independent statistical variables lower than the number of the measured reaction rates, can be used successfully for the solution of the unfolding problem. A great advantage of this method is that the neutron spectrum can be determined when no other real information is available except the reaction rates. The energy resolution of the method is determined by the number of the cross sections and the shapes of the excitation functions. Therefore, the solution is similar to a neutron spectrum measured by a neutron spectrometer with low energy resolution.

If an independent measurement exists for the differential neutron spectrum, there are two possibilities to combine these data with the result of the unfolding calculation:

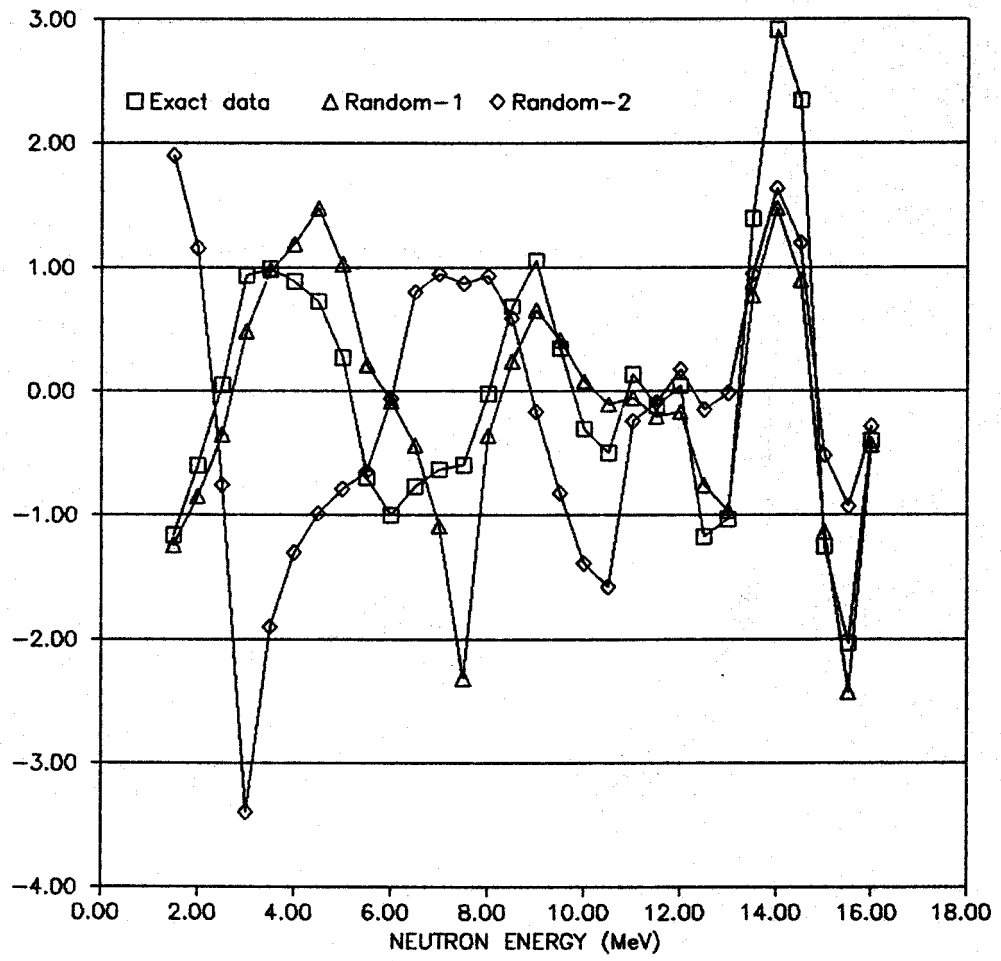

Figure 4. The quantity $(\phi_i-\phi_{io})/\sqrt{N_{ii}}$ in the function of neutron energy for the three data sets.

1. If the covariance matrix of this independent measurement is non-singular, i.e. it is a real measurement, then it can be combined with the solution of the successive approximation method on the basis of the general least squares method and the new improved solution will be:

$$\Phi' = \mathbb{N}_1(\mathbb{N}_1+\mathbb{N}_2)^{-1}\Phi_2 + \mathbb{N}_2(\mathbb{N}_1+\mathbb{N}_2)^{-1}\Phi_1$$
$$\mathbb{N}' = \mathbb{N}_1(\mathbb{N}_1+\mathbb{N}_2)^{-1}\mathbb{N}_2$$

2. If the covariance matrix of the measurement is singular, the usual way of the unfolding by the generalized least squares method can be used. But if the measurement has large errors, the result can be improved by the iterative method described in the present paper.

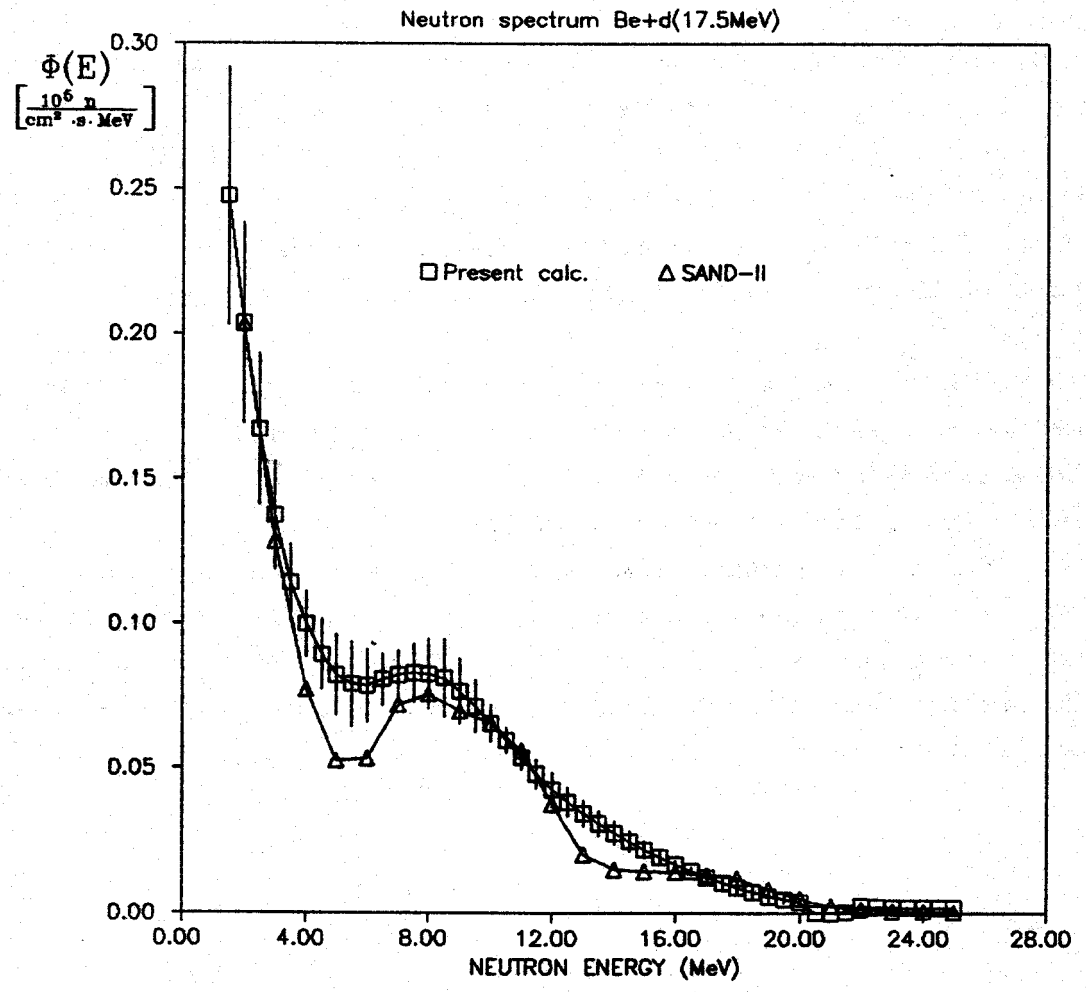

Figure 5. Differential neutron spectrum from the Be+d reaction at 17.5 MeV deuteron energy, calculated by the successive approximation method and the SAND-II unfolding code.

References:

1. Proceedings of the IAEA Consultants' Meeting on the Assessment of the Results of the Real-84 Exercise. INDC(NDS)-190/G+F+R, 1987.
2. M.A. Berzonis, Kh.Ya. Bondars, et al.,"Choice of Activation Detectors for Integral Experiments in the Fusion Reactor Blanket Models," INDC(CCP)-282/GFR, 1988.
3. С.Н. Ежов, В.А. Поярков, "Изучение ядерных реакций в случае немонохроматичецкий пучков" Ядерная Физика Т. 37. вып. 3. 616. 1983.
4. W.N. McElroy et al., "SAND-II A Computer Automated Iterative Method for Neutron Flux Determination by Foil Activation," AFWL-TR-67-41 Vol. I-IV.(1967), p. 368.
5. C.R. Greer, J.A. Halbleib and J.V. Walker, "A Technique for Unfolding Neutron Spectra from Activities Measurements," ISC-RR-67-746, 1967.

6. M. Najzer, B. Glumac, M. Pauko, "Many Channel Spectrum Unfolding," Proc. of 3rd ASTM Euratom Symp. on Reactor Dosimetry, EUR 6813 EN-FR, 1980, Vol. 2., p. 743-750.
7. F.G. Perey, "Spectrum Unfolding by the Least-Squares Method" Proc. IAEA Technical Committee Meeting on the Current Status of Neutron Spectrum Unfolding, Oak Ridge, Tennessee, Oct. 10-12, 1977.
8. D.W. Muir, "A Non-restrictive Derivation of the Generalized Method of Least Squares," Proc. of IAEA Specialists' Meeting on Covariance Methods and Practices in the Field of the Nuclear Data, Rome, Italy,1986, INDC(NDS)-192/L, 1988, p.117.
9. R. Wölfle, S. Sudár, S.M. Qaim, "Determination of Excitation Function of Triton Emission Reaction on Aluminum from Threshold up to 30 MeV via Activation in Diverse Neutron Fields and Unfolding Code Calculations," Nuclear Science and Engineering 91.(1985)162.