A comparison of computer codes for fast neutron dosimetry by the foil technique

Jau Wen Chen

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A COMPARISON OF COMPUTER CODES FOR FAST NEUTRON DOSIMETRY
BY THE FOIL TECHNIQUE

BY

JAU WEN CHEN, 1944-

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ABSTRACT

A comparison of the major codes currently used for fast neutron dosimetry based on the foil technique has been made. These codes are SAND II, SPECTRA and ADMM. The comparison is based upon the deviation of calculated-from-measured activities, the input data decks, the obtained information, and the computer time required.

Four sets of data were used to be compared upon the above four viewpoints, the conclusion reached is that the SPECTRA computer code is the most satisfactory for the UMR Reactor fast neutron spectrum.
ACKNOWLEDGMENTS

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I. INTRODUCTION

Using threshold detectors for the measurement of fast neutron spectra has been a common practice for many years [1], and the method has been improved many times. These techniques are based upon a determination of the specific activity of a detector and from the activity a deduction is made, through knowing the detector response function, of the neutron flux and/or energy distribution which induced the radioactivity.

In the thermal neutron measurements, the characteristic shape of the neutron environment is known and a measurement with a single detector is sufficient to establish the magnitude of the neutron flux. But, many measurements are necessary in epithermal and fast neutron environments where only a general shape of the energy distribution of the neutrons is known. Thus, in these situations the utilization of several activation detectors with different response functions for neutron activation has seen acceptance and is reliable.

The threshold detector technique has the following advantage [4,8]:

1. the threshold detectors are not sensitive to the high gamma fluxes found in reactors,
2. the activation measurement is easy and not very expensive,
3. the small volume and low macroscopic cross-
section of the detectors minimize flux deformations,

4. no connections with the outside of the reactor are required.

The method of interpretation of the activation is described in Section II, whereas Section III will briefly describe the three major codes currently used in this technique. These codes are SAND II, SPECTRA and RDMM. Section IV describes results and conclusions of the comparison of these codes.
II. STATEMENT OF THE PROBLEM

Measurements of in-pile fast neutron spectra are often by threshold detector irradiations. The threshold detector technique gives results usually expressed as normalized activation rates,

\[ A_i = \int_0^{\infty} \sigma_i(E) \phi(E) \, dE \]  

(1)

where \( \sigma_i(E) \) is the energy dependent activity cross-section, \( A_i \) is the reaction rate for a nucleus of the \( i \)'th isotope, and \( \phi(E) \) n/cm\(^2\)-sec-Mev is the time integrated, energy dependent unknown neutron flux.

Three codes, described in the following section, allow the \( \phi(E) \) determination, and we want to compare the three major codes currently used in this technique.

In order to solve Equation 1 and find the flux spectra, two basic principles are used [8]:

1. the total energy range is divided into energy bands;
2. in each energy band a spectral shape is assumed which is predicted by theoretical considerations and calculations.

The criteria of the comparisons will be based upon several items, such as, the relative deviation, the complexity of input data, the obtained information from the output, and the computer time required.
III. REVIEW OF LITERATURE

A number of techniques have been suggested for the solution of Equation 1 for the energy dependent neutron flux. The resulting spectra come in many forms:

1. histogram,
2. piecewise linear,
3. series expansion (e.g., power exponential, orthogonal function),
4. combinations of the above with special physical shapes,
5. combinations of the above with weight functions.

Where histogram or piecewise linear representations are obtained, generally no assumptions are made concerning the spectral shape. In the case of series expansions, this may or may not be true. The spectrum always, however, has a shape characteristic of the expansion functions and weighting functions; and special physical shapes always imply some assumptions about the spectral shape.

The major codes currently used, SAND II, SPECTRA and RDMM, will be discussed as follows:

A. SAND II CODE [2]

The original version of this code gave spurious structure propagated by the iterative method from differential structure in neutron detector reaction cross-sections.
The iterative algorithm used in the SAND II code can be written as:

\[
\phi_j^{(k+1)} = \phi_j^{(k)} \exp(c_j^{(k)}), \quad j=1,2,\ldots,m; \quad (2)
\]

where

\[
c_j^{(k)} = \sum_{i=1}^{n} \frac{w_{i,j}^{(k)} \ln \left( \frac{A_i}{A_i^{(k)}} \right)}{\sum_{i=1}^{n} w_{i,j}^{(k)}}, \quad j=1,2,\ldots,m; \quad (3)
\]

\[
w_{i,j}^{(k)} = \frac{A_{i,j}^{(k)}}{A_i^{(k)}}, \quad j=1,\ldots,m; \quad i=1,\ldots,n; \quad (4)
\]

\[
A_{i,j}^{(k)} = \phi_j^{(k)} \sigma_{i,j}^{(k)} (E_{j+1} - E_j), \quad j=1,2,\ldots,m; \quad i=1,2,\ldots,n; \quad (5)
\]

\[
A_i^{(k)} = \sum_{j=1}^{m} A_{i,j}^{(k)}, \quad i=1,2,\ldots,n; \quad (6)
\]

\[
\phi_j^{(k)} = k^{th} \text{ iterative differential flux over the } j^{th} \text{ energy interval;}
\]

\[
c_j^{(k)} = k^{th} \text{ iterative flux correction term for the } j^{th} \text{ energy interval;}
\]

\[A_i = \text{measured activity for the } i^{th} \text{ detector reaction (extrapolated to saturation and infinite dilution);}
\]

\[A_i^{(k)} = \text{calculated (saturated, infinite dilute) activity for the } i^{th} \text{ detector reaction, based on the } k^{th} \text{ iterative flux spectrum;}
\]

\[A_{i,j}^{(k)} = \text{that portion of } A_i^{(k)} \text{ contributed by neutrons in the } j^{th} \text{ energy interval;}
\]
\[
\sigma_{i,j} = i^{th} \text{ detector reaction cross-section (averaged constant) over the } j^{th} \text{ energy interval;}
\]
\[
E_j = \text{lower energy bound of the } j^{th} \text{ energy interval;}
\]
\[
m = \text{total number of energy intervals (currently 620);}
\]
\[
n = \text{number of detectors used.}
\]

The first attempt to minimize spurious structure was a renormalization of the weighting function to unity quotient of total activity divided by effective range. That is, Equation 5 was replaced by
\[
\tilde{w}_{i,j}^{(k)} = \left(\frac{E_{H,i}^{(k)} - E_{L,i}^{(k)}}{A_{i,j}^{(k)}} / A_{i}^{(k)} \right),
\]
where \(E_{L,i}^{(k)}\) and \(E_{H,i}^{(k)}\) are the 5\% and 95\% "tail" cutoff energies, respectively, for the \(i^{th}\) reaction sensitivity.

The original normalization effectively gave each reaction measurement equal total effect, in some sense, on the total solution flux; thus the new normalization was intended to make each reaction affect the total flux only in proportion to the relative size of the energy region over which it is sensitive. The effect is to reduce the magnitude of those weighting functions which consist mostly of very large resonance peaks over very narrow energy regions so as to reduce the reflections of these peaks in the solution spectrum.
Second, an attempt was made to find some two-parameter analytical form for use as the weighting function, which would describe the sensitivity distribution of a given reaction by means of first and second moments ($\mu$ and $\mu_2$, respectively). The beta distribution was used. The form is:

$$w(x) = x^a (1-x)^b, \quad 0 \leq x \leq 1,$$

where

$$X = (x-x_L)/(x_H-x_L),$$
$$a = (2M^2-M_2(M+1))/(M_2-M^2),$$
$$b = (M-(2-M)M_2)/(M_2-M^2),$$
$$M = (\mu-x_L)/(x_H-x_L),$$
$$M_2 = (\mu_2-x_L(2\mu-x_L))/(x_H-x_L)^2,$$

and $x_L$ and $x_H$ are suitably chosen lower and upper limits, respectively, for $x$.

At last, the method of moving $k$-point $n$th degree polynomial least-squares fitting as being both appropriate and convenient was selected. In this method, each tabulated value of a function is replaced by the value of a polynomial of degree $n$ fitted by standard least-squares techniques to a subrange of $k$ (odd) points, centered (if possible) at the point being modified. Thus, each smoothed value is obtained from a distinct least-squares polynomials except near each end of the
range of the function being smoothed, where the polynomial fitted to the extreme k points is used to smooth the extreme \((k+1)/2\) points. Clearly for any given k, \(n=1\) (straight line) provides the most severe smoothing, and for any given n, smoothing severity increases with increasing k. Thus, for trial purposes, \(n=1\) was chosen for testing various values of k. In general, k is odd, then for least-squares fitting of a straight line to the k points \((x_i,y_i), i=j-\frac{k-1}{2},...,j+\frac{k-1}{2}\). And assume the points are equispaced along the abscissa, that is, for all \(i\), \(x_i - x_{i-1} = d\), and if \(x_i\) is defined by

\[
X = \frac{x_i - x_j}{d} = \frac{(i-j)d}{d} = i-j,
\]

then let \(i_L\) and \(i_H\) be denoted \(j - \frac{k-1}{2}\) and \(j + \frac{k-1}{2}\), respectively.

\[
\sum_{i=i_L}^{i_H} x_i = \sum_{i=i_L}^{i_H} i - \sum_{i=i_L}^{i_H} j
\]

\[
= \frac{(j+\frac{k-1}{2})(j+\frac{k-1}{2}+1)-(j-\frac{k-1}{2}-1)(j-\frac{k-1}{2})}{2} -kj=0, \tag{7}
\]

and

\[
\sum_{i=i_L}^{i_H} x_i^2 = \sum_{i=i_L}^{i_H} i^2 - 2j \sum_{i=i_L}^{i_H} i + \sum_{i=i_L}^{i_H} j^2
\]

\[
= \frac{1}{6} (j+\frac{k-1}{2})(j+\frac{k+1}{2})(2j+k)-(j-\frac{k-1}{2})(j-\frac{k+1}{2})(2j-k)
\]
\[-j(j+\frac{k-1}{2})(j+\frac{k+1}{2})-(j-\frac{k-1}{2})(j-\frac{k+1}{2})+kj^2 = k(k^2-1)/12. \tag{8}\]

Thus, if \(w_x = ax + b\) is fitted to the \(k\) points \((x_i, y_i)\),

where

\[a = \frac{k \sum x_i y_i - \sum x_i \sum y_i}{k \sum x_i^2 - \left(\sum x_i\right)^2} = \frac{12 \sum x_i y_i}{k(k^2 - 1)},\]

\[b = \frac{k \sum x_i^2 \sum y_i - \sum x_i \sum x_i y_i}{k \sum x_i^2 - \left(\sum x_i\right)^2} = \frac{\sum y_i}{k}. \tag{9}\]

where \(i\) from \(j-\frac{k-1}{2}\) to \(j+\frac{k+1}{2}\).

\[w_{x=x_j} = w_{x=0} = \frac{1}{k} \sum_{i=j-\frac{k-1}{2}}^{j+\frac{k-1}{2}} y_i, \quad j=\frac{k+1}{2}, \ldots, m=\frac{k-1}{2}, \tag{10}\]

where \(m\) is the total number of points in the range.

To smooth \(y_j\) for \(j=1, \ldots, \frac{k-1}{2}\), and for \(j=m-\frac{k+1}{2}, \ldots, m\), the straight lines centered about \((\bar{x}(k+1)/2, \bar{y}(k+1)/2)\) and \((\bar{x}m-(k-1)/2, \bar{y}m-(k-1)/2)\) are used respectively. The resultant smoothing forms are:

\[w_{x=x_j} = \frac{1}{k} \left[ \frac{6(2i-k-1)}{k^2-1} \sum_{i=1}^{k} (1-\frac{k+1}{2})y_i + \sum_{i=1}^{k} y_i \right]. \quad j=1, \ldots, \frac{k-1}{2}; \tag{11}\]

and
\[
W_{x=x_j} = \frac{1}{k} \left[ \frac{6(2j-2m+k-1)}{k^2-1} \sum_{i=m-\frac{k-1}{2}}^{m} (i-m+k-1)y_i + \sum_{i=m-\frac{k-1}{2}}^{m} y_i \right]
\]

\[j=m-\frac{k-3}{2}, \ldots, m. \tag{12}\]

The smoothing forms of Eqs. 10 through 12 are based on equidistant abscissa spacing. Since, in the SAND II code, the energy grid is approximately logarithmic between \(10^{-10}\) and 1 Mev, and linearly spaced between 1 and 18 Mev, this smoothing technique provides quasi-logarithmic least-squares smoothing below 1 Mev and rigorous linear least-squares smoothing above 1 Mev. Since it restricts the ends of all weighting functions to be linear and the least-squares line could assume negative values in extreme low and high regions, thus the weighting functions are modified by Eqs. 13 through 15 using for smoothing.

\[
W_{i,j}(k) = \sum_{l=1}^{l_2} A_{i,l}(k)/(l_2-l_1+1)A_i(k), \quad j=2, \ldots, m-1; \quad i=1, \ldots, n; \tag{13}\]

where \(l_1=1\),

\[
= j-\left(\frac{N_S-1}{2}\right), \quad j=\left(\frac{N_S+1}{2}\right), \ldots, \left(\frac{N_S-1}{2}\right), \tag{13a}\]

\[
= 2j-m, \quad j= m-\left(\frac{N_S-3}{2}\right), \ldots, m-1, \tag{13b}\]

and \(l_2=2j-1\),

\[
= j+\left(\frac{N_S-1}{2}\right), \quad j=\left(\frac{N_S+1}{2}\right), \ldots, \left(\frac{N_S-1}{2}\right), \tag{13c}\]

\[
= 2j- m, \quad j= m-\left(\frac{N_S-3}{2}\right), \ldots, \left(\frac{N_S-1}{2}\right). \tag{13d}\]

\[
= j+\left(\frac{N_S-1}{2}\right), \quad j=\left(\frac{N_S+1}{2}\right), \ldots, \left(\frac{N_S-1}{2}\right). \tag{13e}\]
\[ j = (m - \frac{N_S - 3}{2}), \ldots, (m-1); \]  

(13f)

\[ W_{i,1}^{(k)} = \frac{5A_{i,1}^{(k)} + 2A_{i,2}^{(k)} - A_{i,3}^{(k)}}{6A_i^{(k)}}, \]  

(14)

\[ W_{i,m}^{(k)} = \frac{5A_{i,m}^{(k)} + 2A_{i,m-1}^{(k)} - A_{i,m-2}^{(k)}}{6A_i^{(k)}}. \]  

(15)

The influence of the various degree of smoothing, represented by Eqs. 13 through 15, on solution spectra is much as would be expected. The most important observation is that the degree of smoothing (value of \( N_S \)) is a fairly sensitive function of the particular conditions which apply. It is emphasized that the manual spectral smoothing discussed here is very different from the weighting function smoothing. The spectral smoothing will in general change the values of calculated detector activities and may result in a spectrum which is not an appropriate solution. The weighting function smoothing simply affects the iterative procedure, but in no way affects the accuracy of the activity calculations for the eventual solution spectrum.

B. RDMM CODE [3]

This code is based on the group of methods known as 'polynomial' and 'orthogonal' methods [4], because

1. it seems to be the most suitable for the neutron spectral description, since it is not restricted to reactor-type spectra.

2. a development is possible that allows inter-
pretation of the activation data, even when the detectors do not have completely linearly independent cross-sections.

The polynomial method uses as the spectral shape a polynomial in energy having as many terms as there are detectors used multiplied by a chosen weighting function. The orthonormal method uses a series expansion of orthonormal functions. Then

\[ \phi(E) = W(E) \sum_{k=1}^{n} a_k \psi_k \]  

where

- \( n \) = number of detectors,
- \( a_k \) = coefficient constant,
- \( W(E) \) = weighting function,
- \( \psi_k(E) \) = system of function.

In fact, by introducing the Equation 16 into 1, one obtains:

\[ A_i = \sum_{k=1}^{n} a_k S_{ik}, \quad i=1,\ldots,n; \]  

where

\[ S_{ik} = \int W(E) \psi_k(E) \sigma_i(E) \, dE \]  

The following conditions are implicit in the above:

1. It must be possible to use all the available data of activation, independently of their cross-section shapes,
2. The solution must approximate the $A_i$ values in the best possible way, at the same time producing realistic spectral shapes (non-oscillating spectra, no negative-flux values).

Then, we can expand the flux as

$$\phi(E) = \psi(E) \sum_{k=1}^{n} a_k \psi_k(E)$$  \hspace{1cm} (19)

The shape of the spectrum $T1$ used currently (see Table A.2) is described by the following function:

$$\phi(E) = (e^{-2.3E} + .03e^{-0.75E}) e^{-0.5+E}$$

The best approximation to $\phi(E)$ is assumed to be the one minimizing the quadratic form:

$$Q(t; a_1, \ldots, a_t) = \sum_{i=1}^{n} \left( \frac{A_i - \int \phi^t(E) \phi(E) \, dE}{A_i} \right)^2$$  \hspace{1cm} (20)

where $t=1,2,\ldots,n$.

$$\phi^t(E) = \psi(E) \sum_{k=1}^{t} a_k \psi_k(E)$$

if $m = \text{optimum value of the expansion terms}$,

$$\phi^m(E) = \text{related approximation},$$

$n = \text{number of detectors}$. Then the only condition is $m \leq n$.

The requirement of minimum $Q(t)$ is

$$\frac{\partial Q(t)}{\partial a_j} = -2 \left( \sum_{i=1}^{n} r_{ij} - \sum_{i=1}^{n} r_{ij} \sum_{k=1}^{t} a_k r_{ik} \right) = 0$$  \hspace{1cm} (21)

\hspace{1cm} j=1,\ldots,t
where \( r_{ij} = \frac{S_{ij}}{A_i} \), and leads to the matrix form:

\[
R^T R a = R^T e,
\]

(22)

where:

\[
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_t
\end{pmatrix}
= \begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_t
\end{pmatrix}
\begin{pmatrix}
1 \\
1 \\
\vdots \\
1
\end{pmatrix}
\begin{pmatrix}
r_{1,1} & \cdots & r_{1,t} \\
\vdots \\
\vdots \\
r_{n,1} & \cdots & r_{n,t}
\end{pmatrix}
\]

\( R^T \) indicates the transpose of the matrix \( R \).

Errors are caused by the following:

1. inaccuracy of the hypothesis expressed by Equation 19,
2. round-off errors in the numerical procedures,
3. experimental errors in the activation rates,
4. inaccuracy in the values of the cross-sections.

With regard to the last two points, the form of standard errors are

\[ A_i \pm h_i A_i. \]

and

\[ \sigma_i(E) \pm k_i \sigma_i(E) \]

where \( h_i \) and \( k_i \) will be suitably chosen then the evaluation of errors in the computed spectral shape is the form

\[ \phi(E) \pm e(E) \phi(E) \]
where \( e(E) \) is the percent statistical error.

The numerical tests suggest the following:

1. The errors have an oscillating character that is related to the poles and zeros of the functions chosen for the series expansion.

2. The errors grow linearly with the errors in the input data.

3. The error grows when the number of detectors used is reduced.

4. The error grows when the number of terms in expansion increases, this fact may be related to the observations about the stability of the system.

5. The statistical error appears greatest in the regions where the solutions approximate the test spectrum in the worst way.

The role of the weighting function, \( W(E) \), is important in the solution of the problem, because the expression of Equation 19 may be interpreted in the following sense: the unknown flux is obtained from the shapes of the function \( W(E) \) through the deformation described by the series expansion.

Comment 3 is important since, in order to obtain good results, it is necessary to use the maximum number of available detectors.

Comment 4 suggests a reduction in the number of
expansion terms used; but this may be in contrast with the choice suggested by the minimization of \( Q \). For example, minimum value of \( Q \) may suggest the choice \( m=6 \), but with \( m=4, 5 \) very similar; then the solution must be chosen between \( \phi^4, \phi^5, \phi^6 \).

If the input errors are 2.5\%, \( \phi^5 \) and \( \phi^6 \) seem to be equivalent from the point of view of the reliability. But, if the input errors are increased to 5\%, \( \phi^4 \) is preferred, because its statistical errors are lower.

C. SPECTRA CODE [5,6]

In the SPECTRA code, the flux is approximated by piecewise linear functions of energy and Equation 1 is reduced to the matrix form

\[
A = C\phi
\]  

where \( A \) is an \( n \times 1 \) vector whose entries are the measured activities, \( \phi \) is an \( m \times 1 \) vector whose entries are the desired flux values, and \( C \) is an \( n \times m \) matrix whose elements are certain integrals of the cross-sections. The differential flux \( \phi(E) \) in the interval \( E_i \) to \( E_{i+1} \) is given by

\[
\phi(E) = \phi_{i+1} \left( \frac{E - E_i}{E_{i+1} - E_i} \right) + \phi_i \left( \frac{E_{i+1} - E}{E_{i+1} - E_i} \right). \tag{24}
\]

It is assumed that there is no differential flux below \( E_1 \) and that the differential flux value at \( E_m \) is zero, that is, \( \phi_m = 0 \), and
In order to solve Equation 23, it is assumed that the first $n \times n$ submatrix of $C$ is nonsingular, where $n$ is the rank of $c$. If the calculated activities are denoted by $A_c$, then the least squared difference, $E$, between the measured activity, $A$, and the calculated activity is given by $E = (A_c - A)^T(A_c - A)$. The function $E$ is minimal with respect to $\phi_c$ when 

$$
\frac{\partial E}{\partial \phi_c} = 0 \text{ and } \frac{\partial^2 E}{\partial \phi_c^2} \text{ is positive definite with } A_c = C\phi_c,
$$

$$
\frac{\partial E}{\partial \phi_c} = 2(C^T C \phi_c - C^T A_c) = 0, \text{ and, if } C^T C \text{ is nonsingular, the desired solution is } \phi_c = (C^T C)^{-1}C^T A_c. \text{ When } m > n, \text{ the matrix } C^T C \text{ is singular and a unique solution is the least squared sense does not exist.}
$$
We defined a new error function as

\[ E_1 = (A_c - A)^T (A_c - A) + (\emptyset - \emptyset_o)^T (\emptyset - \emptyset_o), \quad (27) \]

where \( \emptyset_o \) is an approximate solution. Differentiating the new error function with respect to \( \emptyset_1 \) and equating to zero yields

\[ \frac{\partial E_1}{\partial \emptyset} = 2C^T (A_c - A) + 2I^T (\emptyset - \emptyset_o) = 0 \quad (28) \]

and \[ \frac{\partial^2 E_1}{\partial \emptyset^2} = C^TC + I. \] If \( \frac{\partial^2 E_1}{\partial \emptyset^2} \) is positive definite, a unique solution of equation (28) exists which minimizes the error function. Since, if \( B \) is an \( m \times m \) positive (semi-)definite matrix and \( F \) is an \( m \times m \) diagonal matrix with non-negative entries, then \( B + F \) is positive definite, thus, the matrix \( C^TC + I \) is positive definite.

Suppose \( C^T (\emptyset - A) = 0 \), the matrix \( C = (X, Y) \) where \( X \) is an \( n \times n \) nonsingular matrix and

\[ C^T = \begin{pmatrix} X^T \\ Y^T \end{pmatrix}. \] Now \( X^T \) has an inverse and \([ (X^T)^{-1} , 0 ] \begin{pmatrix} X^T \\ Y^T \end{pmatrix} = C^T A = 0 \), which implies \( C^T A = 0 \), that is, the vector \( \emptyset \) is a solution to the equation \( C^T \emptyset = A \). If we define the matrix

\[ F = (C^T C + I)^{-1} \quad (29) \]

\[ B = FC^T A \quad (30) \]

then we obtain an iterative algorithm,

\[ \emptyset_{i+1} = B + F\emptyset_i. \quad (31) \]

Repeated applications of the algorithm yields the
matrix series

\[ \phi_n = (I + F + \ldots + F^{n-1}) B + F^n \phi_0, \]  

(32)
since the matrix \( C^T C \) is positive definite which implies the eigenvalues of \( C^T C + I \) are greater than 1. Thus the eigenvalues of \( F \) are between zero and one, which implies \( F^n \to 0 \) and \( I + F + F^2 + \ldots \) converges to \( (I + F)^{-1} \), thus obtaining the solution \( \phi = (I - F)^{-1} B \). From the definition of \( F \), we have \( F(C^T C + I) = I \to I - F = F C^T C \to \phi = (F C^T C)^{-1} B = (F C^T C)^{-1} F C^T A = I \phi \), where \( \phi \) is the unique solution of \( C^{-1} A \).

Since the error \( E_1 \) is strictly monotonically decreasing if \( \phi_0 \) is not a solution to \( A = C \phi \), then we can the iterative method to solve the Equation 23. Because \( \lim_{n \to \infty} E\phi_n = 0 \); \( \lim_{n \to \infty} \phi_n \) exists and is a solution to \( A = C \phi \).

The methods of SPECTRA are based on the above theory. Experience have led to several observations concerning the use of the proposed method. At first, it should be recognized that in the overdetermined condition, the solution values one obtains are somewhat dependent upon the trial solution. This characteristic is, of course, by choice since the method is designed to take advantage of any additional physical information one has about the spectral distribution. This physical information may be only qualitative; for example, the
spectrum might be thought to be a softened fission spectrum, a fusion spectrum; or one might have an actual crude theoretical spectrum which can be used. Secondly, errors in activation measurements, as in other techniques for solving this system of equations, can be magnified in the calculated flux. That is, a fractional error in one of the activities can cause a much larger error in one or more of the discrete differential flux values rather than distributing the error over the entire region of sensitivity. Thirdly, even without error in the activities, the calculated flux will sometimes show structure about the actual spectral shape due to the manner in which the initial trial function is perturbed by the detector response functions. This is particularly noticeable when it is necessary for the code to modify the trial flux considerably to obtain a solution.
IV. RESULTS AND DISCUSSION

There are four sets of activities presented, three measured and one estimated. The first set contains 10 foils. These reactions are In\textsubscript{115}(n,n')In\textsubscript{115m}, Mg\textsubscript{24}(n,p)Na\textsubscript{24}, Ni\textsubscript{58}(n,p)Co\textsubscript{58}, Th\textsubscript{232}(n,f)FP, U\textsubscript{235}(n,f)FP, U\textsubscript{238}(n,f)FP, Al\textsubscript{27}(n,He)Na\textsubscript{24}, Cu\textsubscript{63}(n,G)Cu\textsubscript{64}, Fe\textsubscript{54}(n,p)Mn\textsubscript{54}, Au\textsubscript{197}(n,G)Au\textsubscript{198}. These are the test data of the SAND II code. The second set has 5 foils, that is, Al\textsubscript{27}(n,p)Mg\textsubscript{27}, Al\textsubscript{17}(n,He)Na\textsubscript{24}, Cu\textsubscript{63}(n,G)Cu\textsubscript{64}, Fe\textsubscript{56}(n,p)Mn\textsubscript{56}, Ni\textsubscript{58}(n,p)Co\textsubscript{58}. These activities are obtained from UMR Reactor. The third and fourth sets contain the same 7 foils. These are Al\textsubscript{27}(n,He)Na\textsubscript{24}, In\textsubscript{115}(n,n')In\textsubscript{115m}, Al\textsubscript{27}(n,p)Mg\textsubscript{27}, Fe\textsubscript{54}(n,p)Mn\textsubscript{54}, Fe\textsubscript{56}(n,p)Mn\textsubscript{56}, Mg\textsubscript{24}(n,p)Na\textsubscript{24}, Ni\textsubscript{58}(n,p)Co\textsubscript{58}. The former are from Henry A. Till [7]. Because all program codes got very poor results using these activity data, the fourth set is estimated values based on the results using the third set run in the SAND II code.

In order to fit these four sets of data, the first thing must be to obtain the input (or trial) spectrum. The differential neutron spectrum of the UMR Reactor at core position C3 (see Appendix F or Ref. 7) is used in second, third and fourth sets to fit all the three computer codes.

The highest energy value in the SAND II test data
is only 3 Mev, but it should be generated up to 18 Mev. One way to get this entire spectrum is from the first approximation spectrum in the SAND II code. It is easily seen that it is reliable because the errors between the input flux and the first approximation flux are all less than 5 percent.

The criteria of the comparison will be based on the computer time required, the calculated-to-measured activity ratio, the complexity of input data, and the obtained information from the output.

A. COMPUTER TIME REQUIRED

The RDMM code is the best one based on this criteria (see Table 1). Both SAND II and SPECTRA codes have free field input and iterative processes that use much time in data transmissions and iterations. The plot subroutine GRAF in the SAND II code uses nominally 120 minutes or $36.- per case on the Calcomp Model 556 Digital Incremental Plotter. A major portion of this plotting time is occupied by the drawing of variable log-log grid.

B. CALCULATED-TO-MEASURED ACTIVITY RATIOS

There seems to be little difference between the three codes in this category. The RDMM code results in Table 2 are from the approximation order 6 of Monte Carlo histories. In the 5-foil case, the order of the
approximation polynomial, $\text{MAX}=6$, is greater than the number of foils, $\text{NS}=5$. In the case of 10 foils, the reason for these ratios of foils $\text{Au197}(n,G)\text{Au198}$ and $\text{Cu63}(n,G)\text{Cu64}$ poor results in the RDMM and SPECTRA codes is the former foil activity sensitivity range being from $4.75 \times 10^{-6}$ to $3.4 \times 10^{-2}$ Mev and the latter foil activity sensitivity range being from $5.75 \times 10^{-4}$ to $0.12$ Mev. Perhaps, these two codes do not have enough information on cross-sections in this range. These are gamma reactions, and the cross-section for the gamma reaction is generally very low in the fast neutron range.

In the third case with 7 foils, the RDMM code had one negative ratio for the $\text{Al27}(n,p)\text{Mg27}$ reaction, and the SPECTRA code had one for the $\text{In115}(n,n')\text{In115m}$ reaction. From Equation 1, recall that the calculated activation rate is defined as the summation of the product of neutron cross-section and neutron differential flux. We use the $\text{Al27}(n,p)\text{Mg27}$ reaction to illustrate the reason why these ratios sometimes were negative. Because the RDMM code gave high negative flux within a wide energy range from 3.1 to 7.9 Mev (see Figures 5 and Appendix C), then, the calculated activation rate became a negative value.

The relationships of activation rates between the codes should be used carefully (see Appendix B). Some recommendations in using data are listed in Appendix D.
C. COMPLEXITY OF INPUT DATA

It seems to be that the SPECTRA code is the best one based on this criteria (see Appendix A). The RDMM code requires hundreds of cards for cross-section information in each case. If someone were to run two cases with the same foils in each, then he should duplicate these data decks. However, it seems to be inefficient and ambiguous work.

The SAND II code is only slightly more complicated than the SPECTRA code. One thing has to be noticed in the SAND II and SPECTRA codes is that the foil name used must be the same as the foil name in the library file (see Appendix C). One should notice the relations among the codes.

D. OUTPUT

There are detailed descriptions for the output forms of each code in Appendix B.

In order to compare the three codes, four sets of data were run in each computer code. These results were then plotted by the Calcomp Model 556 Digital Incremental Plotter in the same unity. (see Figures 1 to 8)

The reasons for any discontinuity in the flux curve are: the flux is extremely low, or the flux has a negative value. The first happened nine to ten in the SAND II code. The second always happened in the RDMM and SPECTRA
codes, but, never occurred in the SAND II code. The SAND II code never yielded a negative flux values.

From Figures 1 and 2, the SPECTRA code appears to be the worst one, but it still agrees at the high energy range, say above 9 Mev, after the use of subroutine REPETE. In the Figures 3 and 4, the RDMM results are nearly perfect except there is not indicated peak at 14-15 Mev. The results of subroutine LIMIT in the SPECTRA code seems to be better than the RDMM code above 7 Mev. It is interesting to note, if we connect two discontinuous points in the curve of LIMIT these seems to be a good fit of the trial flux. The differential flux obtained from the SAND II code has an obvious peak at 6 Mev, but this peak does not occur in Figures 5 or 7 (both were calculated with the same trial flux), so that this peak is not real. From Figure 5, it seems that no code could fit the trial flux due to the large standard deviation of activation rate. But the RDMM and SPECTRA codes seem good in the high energy range, say above 9 Mev.

In Figures 7 and 8, the results from subroutine LIMIT and REPETE of SPECTRA code are very reasonable, especially, at the high energy range. And if we use three or more points smoothing method, we could get a good result.

With reference to the differential flux or the
integral flux, the RDMM and SPECTRA codes seem better than the SAND II code. All in all, it could be said that the SPECTRA code is better than the other two for the UMR Reactor neutron spectrum.
## Table 1
Computer Time Required Comparison

<table>
<thead>
<tr>
<th></th>
<th>SAND II</th>
<th></th>
<th>RDMM</th>
<th></th>
<th>SPECTRA</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time</td>
<td>Cost</td>
<td>Time</td>
<td>Cost</td>
<td>Time</td>
<td>Cost</td>
</tr>
<tr>
<td>Linkedit (average)</td>
<td>24.11</td>
<td>$0.84</td>
<td>10.37</td>
<td>$0.36</td>
<td>19.80</td>
<td>$0.69</td>
</tr>
<tr>
<td>GO</td>
<td>Minimum</td>
<td>3:30.00</td>
<td>1:40.00</td>
<td>$3.50</td>
<td>7:20.00</td>
<td>$15.40</td>
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<tr>
<td></td>
<td>Normal</td>
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<td>1:50.00</td>
<td>$3.90</td>
<td>12:00.00</td>
<td>$25.20</td>
</tr>
<tr>
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<td>$36.00</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Total</td>
<td>6:00.00</td>
<td>$48.40</td>
<td>2:00.00</td>
<td>$4.20</td>
<td>12:20.00</td>
<td>$25.90</td>
</tr>
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<td>Test</td>
<td>Reaction</td>
<td>SAND II</td>
<td>RDMM</td>
<td>SPECTRA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>---------</td>
<td>------</td>
<td>---------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 Foils</td>
<td>Al27(n,He)Na24</td>
<td>1.06997</td>
<td>0.97485</td>
<td>0.99999</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Au197(n,G)Au198</td>
<td>1.00090</td>
<td>0.29267</td>
<td>0.50101</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cu63(n,G)Cu64</td>
<td>1.00180</td>
<td>0.62646</td>
<td>1.20329</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fe54(n,p)Mn54</td>
<td>0.92894</td>
<td>0.76501</td>
<td>1.00049</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In115(n,n')In115m</td>
<td>1.09027</td>
<td>1.22863</td>
<td>0.99801</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mg24(n,p)Na24</td>
<td>0.94313</td>
<td>1.04523</td>
<td>0.99998</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ni58(n,p)Co58</td>
<td>0.91550</td>
<td>1.25435</td>
<td>0.99955</td>
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<tr>
<td></td>
<td>Th232(n,f)FP</td>
<td>1.09230</td>
<td>0.77167</td>
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<td>U235(n,f)FP</td>
<td>1.00311</td>
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<td></td>
<td>U338(n,f)FP</td>
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<td>5 Foils</td>
<td>Al27(n,He)Na24</td>
<td>1.57704</td>
<td>1.00000</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Al27(n,p)Mg27</td>
<td>1.92790</td>
<td>1.00000</td>
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<tr>
<td></td>
<td>Cu63(n,G)Cu64</td>
<td>1.13186</td>
<td>1.00000</td>
<td>0.81726</td>
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Table 2 (continue)
Calculated-to-Measured Activity Ratios

<table>
<thead>
<tr>
<th>Test</th>
<th>Reaction</th>
<th>SAND II</th>
<th>RDMM</th>
<th>SPECTRA</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 Foils (continue)</td>
<td>Fe56(n,p)Mn56</td>
<td>0.48237</td>
<td>1.00000</td>
<td>1.00324</td>
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<tr>
<td></td>
<td>Ni58(n,p)Co58</td>
<td>1.12271</td>
<td>1.00000</td>
<td>1.00112</td>
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<tr>
<td>7 Foils Version III</td>
<td>Al27(n,He)Na24</td>
<td>0.95193</td>
<td>1.00104</td>
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<td>1.01184</td>
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<td>1.00268</td>
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<tr>
<td></td>
<td>Fe54(n,p)Mn54</td>
<td>1.04833</td>
<td>0.99092</td>
<td>1.00435</td>
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<td>Fe56(n,p)Mn56</td>
<td>0.97286</td>
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<td></td>
<td>In115(n,n')In115m</td>
<td>1.02020</td>
<td>1.00009</td>
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<tr>
<td></td>
<td>Mg24(n,p)Na24</td>
<td>0.95548</td>
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<td>Ni58(n,p)Co58</td>
<td>1.04976</td>
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<td>7 Foils No Version</td>
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<td></td>
<td>Al27(n,p)Mg27</td>
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<td>Fe54(n,p)Mn54</td>
<td>833.33333</td>
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<td>1.02572</td>
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</table>
Table 2 (continue)
Calculated-to-Measured Activity Ratios

<table>
<thead>
<tr>
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<th>Reaction</th>
<th>SAND II</th>
<th>RDMM</th>
<th>SPECTRA</th>
</tr>
</thead>
<tbody>
<tr>
<td>7 Foils</td>
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<td>0.02445</td>
<td>0.00017</td>
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<tr>
<td>No Version</td>
<td>In115(n,n')In115m</td>
<td>1.29049</td>
<td>0.87005</td>
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<tr>
<td>(continue)</td>
<td>Mg24(n,p)Na24</td>
<td>22.37136</td>
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<td>Ni58(n,p)Co58</td>
<td>14.94768</td>
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Figure 1. Neutron differential spectrum for 10 foils.
Figure 2. Neutron integral spectrum for 10 foils.
Figure 3. Neutron differential spectrum for 5 foils.
Figure 4. Neutron integral spectrum for 5 foils.
Figure 5. Neutron differential spectrum for 7 foils, no version.
Figure 6. Neutron integral spectrum for 7 foils, no version.
Figure 7. Neutron differential spectrum for 7 foils, version III.
Figure 8. Neutron integral spectrum for 7 foils, version III.
V. CONCLUSIONS

In the preceding section, we have compared the three codes from four viewpoints, that is, computer time required, the calculated-to-measured activity ratios, complexity of input data, and information obtained from the output.

Considering the computer time saving, the RDMM code appears to be the optimal code. The RDMM code yields satisfactory results, especially at the high values. We could extrapolate the curve from high energy to low energy. But, it does not follow any peaks in the trial flux. Perhaps, this is not serious in the case of narrow peak widths.

For satisfying the criteria of the simplest data input, the best output results, and the activity ratios, the SPECTRA code appears to be the best one among these three computer codes. Although the SPECTRA code takes much computer time, it still costs less than the SAND II code if the latter is run under a plotting situation.
VI. RECOMMENDATIONS

The scope of the present codes did not permit all the effort which is known to be required to optimize the computer codes. Several areas of effort are recommended below which will either increase the codes’ utility or correct current weaknesses. No indication of priority is intended in the order of discussion.

A. SAND II CODE

The program should be modified to monitor each iteration. Currently, if the time specified by the user in the limit card is exceeded, execution terminates with no further output, essentially wasting the entire run. The provision should be included to initiate step printout of running results (specially, at the fast neutron region) such as in the RDMM code.

A study should be initiated to accelerate toward the solution using some well-known successive iterative process such as, say, Aiken's $\delta^2$ procedure [9]:

$$\phi_j^{(0)}' = \frac{\phi_j^{(k+1)}\phi_j^{(k-1)} - (\phi_j^{(k)})^2}{\phi_j^{(k+1)} + \phi_j^{(k-1)} - 2\phi_j^{(k})}, \quad j=1, \ldots, m$$

This may result in significant savings in execution time.

It should be reprogrammed in the plot subroutine GRAF to plot the marginal line with log incremental grid indicated by tic marks in place of the complete log-log plots. This should reduce the plotting time.
from nominally 120 minutes to 20 minutes.

B. RDWM CODE

The available program should be written to read the foil cross-section information from a tape. This procedure would involve substantial reprogramming of the code, but it would result in effectively simplifying the data input.

The subroutine PESI should be suitably changed in accordance with the shape of neutron spectrum used. This may result in significant spectrum responses.

C. SPECTRA CODE

The iteration process should be modified to save executive time in subroutine REPZTE.
APPENDIX A

DATA FORMAT USED IN COMPUTER CODES

A.1 SAND II CODE

All input data cards are read by SAND II code using subroutine VIF (except the first user's name card) and are therefore free from location and spacing format. The following abbreviations and symbols are used:

[ ] select one;
( ) omit if not need or desired;
n integer number
x "real" or "floating point" number;
a alphameric character.

section -1: user's name, one card. Format: 5A4.
section 0: number of cases, one card.

n CASES

This card is to included only once, at the beginning of the entire data deck for a run.

section 1: title cards, as many cards as desired.

Taaa......aaa......
" " " "

section 2: type of run, and type of activity measurement, one card.

[ ITERATION ]
[ ACTIVITY ] (TIME INTEGRATED)

section 3: one card specifying number of foils, plus
one card for each foil.

\[ n \text{ FOILS} \]
\[ \text{aaa}\ldots \text{a} \] (CADMIUM \( x \)) (BORON \( x \)) (GOLD \( x \))

section 4: for ITERATION RUN only: measured activities, as many cards as needed.

\[ \text{ACTS} \quad x \quad x \quad x \quad x \quad \ldots \]
\[ " \quad " \quad " \quad " \quad " \]

section 5: spectrum form, one card.

\[ \text{SPECTRUM} \quad \begin{bmatrix} \text{LIBRARY (n)} \\ \text{FUNCTION n} \\ \text{TABULAR} \end{bmatrix} \]

section 6: for TABULAR SPECTRUM INPUT only: spectrum tabulation, as many cards as needed.

\[ n \text{ POINTS} \]
\[ \text{ENER} \quad x \quad x \quad x \quad x \quad \ldots \]
\[ " \quad " \quad " \quad " \quad " \]
\[ \text{FLUX} \quad x \quad x \quad x \quad x \quad \ldots \]
\[ " \quad " \quad " \quad " \quad " \]

section 7: for ITERATION RUN only: solution parameters, three cards.

\[ \text{LIMIT n} \]
\[ \text{DEVIA\ldots ION x} \]
\[ \text{DISCARD x} \]

section 8: extrapolation forms and normalization energy, three cards.

\[ \text{LOW END} \quad \begin{bmatrix} E \\ \text{SQRTE} \\ \text{THERMAL (x)} \end{bmatrix} \]
\[ \text{HIGH END} \quad \begin{bmatrix} \text{FISSION} \\ \text{FUSION} \end{bmatrix} \]
NORM \( \times \)

section 9: auxiliary output, one card.
(NO) (PLOT) (NO) (CARDS)

section 10: for ITERATION RUN only: structure retardation, one card.
SMOOTH \( n \)

A.2 RDMM CODE

RDMM is the only code to use format for the input data.

section 0: number of case, one card. Format: 10I6

section 1: title cards, two cards. Format: (9A8)

section 2: NS, NP, NPP card. Format: 10I6
NS = number of detectors, \( n \)
NP = number of points in which the \( \sigma(E) \)
are tabulated
NPP = step of the print-out results

section 3: MIN, MAX card. Format: 10I6
Minimum and maximum order for approximated polynomial. MAX \( \leq n \).

section 4: number of Monte Carlo histories for each approximation order. Format: 10I6

section 5: \( E(1), H \) card. Format: 3E10.6
\( E(1) \) = the first energy value in which the \( \sigma_i(E) \) are tabulated (Mev).
\( H \) = step of the energy tabulation (Mev).
section 6: SIGNME(I). Format: 9A8. One card for the name of foil;
SIGMA(J). Format: 40X,F10.3/(5F10.3) cross-section of the foil I expressed in milli-barn for J=1,NP

section 7: activities and relative standard error on the A and SIGMA.
Format: 3E10.6

section 8: coef. of polynomial formula. Format: 8F10.0

section 9: auxiliary card, scale factor SCALE, and initial random digit IX. Format: E15.3,18

A.3 SPECTRA CODE
SPECTRA code is a "free field" input program (i.e., data fields are not determined by specified columns of a data card. For SPECTRA code, data should be punched in columns 1-72 and data fields are split by commas.

The following is the RUN Mode:
section 0: mode card, one card
RUN
This card is at the beginning for each case.
section 00: title cards, two cards
section 1: contains 5 fields, IFOIL, IENER, MODE, ERRE and MITE, in one card.
IFOIL = number of foils;
IENER = the total number of flux values including both endpoints;
MODE = 0 LIMIT only,
1 REPETE only,
2 both LIMIT and REPETE,
3. ACTIVITY RUN;
ERRE = the required tolerance;
MITE = limit number for iteration.

section 2: contains 2*IENER fields in increasing order of energy with the form energy value, flux value, energy value, flux value, etc.

section 3: contains 3 fields, ITYPE, AC, BI. One card for one foil.
ITYPE = name of the foil;
AC = activation rate;
BI = weight factor.

Table A.1 shows the 5 foils set of data used in SAND II code, Table A.2, A.3, in RDMM and SPECTRA code, respectively.
Table A.1. SAND II Code 5 Foils Data Set

CHEN JAU WEN
1 CASES
T TEST TO USE UMR REACTOR NEUTRON FLUX SPECTRUM AT CORE POSITION C-3
T
ITERATION
5 FOILS
NI58P CADMIUM 0.0508
CU63G CADMIUM 0.0508
FE56P CADMIUM 0.0508
AL27P CADMIUM 0.0508
AL27A CADMIUM 0.0508
SPECTRUM TABULAR
91 POINTS
ENER 1.2 4.6 8. 1 1.2 1.4 1.6 1.8 2 2.2 2.4 2.6 2.8 3 3.2 3.4 3.6 3.8 4
ENER 4.2 4.4 4.6 4.8 5 5.2 5.4 5.6 5.8 6 6.2 6.4 6.6 6.8 7 7.2 7.4 7.6 7.8
ENER 8 8.2 8.4 8.6 8.8 9 9.2 9.4 9.6 9.8 10 10.2 10.4 10.6 10.8 11 11.2 11.4
ENER 11.6 11.8 12 12.2 12.4 12.6 12.8 13 13.2 13.4 13.6 13.8 14 14.2 14.4 14.6
ENER 14.8 15 15.2 15.4 15.6 15.8 16 16.2 16.4 16.6 16.8 17 17.2 17.4 17.6
ENER 17.8 18
FLUX 1.35+8 3.39+8 2.94+7 2.45+7 2.09+7 1.80+7 1.56+7 1.36+7
FLUX 1.19+7 1.04+7 9.16+6 8.04+6 7.05+6 6.19+6 5.43+6 4.77+6 4.18+6 3.66+6
FLUX 3.21+6 2.81+6 2.46+6 2.15+6 1.88+6 1.64+6 1.44+6 1.26+6 1.10+6 0.96+5
FLUX 8.34+5 7.27+5 6.34+5 5.52+5 4.81+5 4.19+5 3.64+5 3.17+5 2.76+5 2.4+5
FLUX 2.09+5 1.81+5 1.57+5 1.37+5 1.19+5 1.03+5 0.95+4 0.89+4 0.83+4 0.77+4 0.71+4 0.65+4 0.6+4 0.55+4
FLUX 5.07+4 4.4+4 3.81+4 3.3+4 2.86+4 2.48+4 2.15+4 1.86+4 1.61+4 1.4+4
FLUX 1.21+4 1.05+4 0.96+4 0.86+4 0.76+4 0.67+4 0.59+4 0.52+4 0.46+4 0.4+4
FLUX 2.45+3 2.0+3 1.57+3 1.3+3 1.05+3 0.9+3 0.8+3 0.7+3 0.6+3 0.5+3 0.4+3
FLUX 424. 366. 316. 273. 236. 203. 175. 151.
Table A.1. SAND II Code 5 Foils Data Set (continue)

LIMIT 25
DEVIATION 5
DISCARD 100.0
LOW END E
HIGH END FISSION
NORM 1.0-10
NO PLOT, NO CARDS
SMOOTH 1
Table A.2. RDMM Code 5 Foils Data Set

1 CASES
I AM TESTING THIS CODE WITH THE SPECTRUM T1 BY UMRR SPECTRUM
RUN FOR ALTERNATE DECK USING 5 DETECTORS FOR SPECTRUM T1

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<td>100</td>
<td>100</td>
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</tbody>
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<th>0.0</th>
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Table A.2. RDMM Code 5 Foils Data Set (continue)

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</tr>
</tbody>
</table>

CU63G

*** 37 cards for cross-section ***

FE56P

*** 37 cards for cross-section ***

AL27P

*** 37 cards for cross-section ***

AL27A

*** 37 cards for cross-section ***
Table A.2. RDMM Code 5 Foils Data Set (continue)

<table>
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<tr>
<th>Code</th>
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<th>CU63G</th>
<th>FE56P</th>
<th>AL27P</th>
<th>AL27A</th>
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<td>.05</td>
<td>.05</td>
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</table>
Table A.3. SPECTRA Code 5 Foils Data Set

RUN
UMR REACTOR FAST NEUTRON SPECTRUM AT CORE POSITION C-3
5 FOILS, 33 POINTS, LIMIT AND REPETE RUN 2,000 ITERATIONS
5, 33, 2, 1.0E-3, 2000
,.01, .0, .1, 2.25E5, .4, 8.2E5, 1., 4.08E5, 1.6, 2.6E5, 2.3, 1.63E5,
3., 1.03E5, 3.6, 6.97E4, 4.3, 4.38E4, 5., 2.73E4, 5.6, 1.83E4, 6.3,
1.13E4, 7., 6983., 7.6, 4600., 8.3, 2817., 9., 1717., 9.6, 1123.,
10.3, 681., 11., 413., 11.6, 268., 12.3, 162., 13., 97.8, 13.6, 63.3,
15.8, 16.2, 9.48, 17., 5.02, 17.2, 2.7, 18., .0
AL27(NHE)NA24 , 93.247 , .2
AL27(NP)MG27 , 59565.2 , .2
CU63(NG)CU64C40 , 330428. , .2
FE56(NP)MN56 , 2885.71 , .2
NI58(NP)CO58 , 164.328 , .2
ENDEND
APPENDIX B

RELATIONS FOR ACTIVITIES IN COMPUTER CODES

The most important information in each of the computer codes used are the activation rates.

The unit of activity in the SAND II code is dis/sec-nucleus. But, for numerical reasons, the order of magnitude must be in the range $10^{-3}$ to $10^3$ in the RDMM code. If the cross-sections are given in millibarns, then a scale factor of $10^{19}$ is usually used for the activities as in the SAND II data. Therefore, a scale factor of $10^8$ must be applied to the results in order to obtain differential flux values in the usual unit, $n/cm^2$-sec-Mev, and integral flux values in $n/cm^2$-sec.

In the SPECTRA code, the activity per unit mass (dis/min-gm) is used. If the cross-section $\sigma_k$ data is in barns, then the activity in the SPECTRA code is scaled by $60*N_0 \lambda/A$ as in the SAND II code, where $N_0$ is the Avogadro's number, $\lambda$ is the decay constant in min$^{-1}$, and $A$ is the atomic weight.
APPENDIX C

CROSS-SECTION INFORMATION USED IN COMPUTER CODES

SAND II and SPECTRA each contain a library of threshold cross-sections for 34 and 29 foil reactions, respectively.

The short reaction names in the SAND II library cross-section file named CSTAPE are as follows:

1. NI58P
2. PU239F
3. SC45G
4. NA23G
5. TH232G
6. U238G
7. AU197G
8. CO59G
9. IN115G
10. MN55G
11. CU63G
12. U238F
13. TH232F
14. ZN64P
15. FE54P
16. S32P
17. SI28P
18. S34A
19. MG24P
20. CL35A
21. NI582
22. I1272
23. ZR902
24. TI46P
25. TI47P
26. TI48P
27. CU632
28. P31P
29. FE56P
30. AL27P
31. NP237F
32. U235F
33. AL27A
34. IN115N
The reaction names in the SPECTRA library cross-section file named SPELIB are as follows:

1. \( \text{AL27(N HE)NA24} \) 2. \( \text{AL27(N P)MG27} \)
3. \( \text{AU197(N G)AU198C} \) 4. \( \text{CL35(N HE)P32} \)
5. \( \text{CO59(N G)CO60C40} \) 6. \( \text{CU63(N 2N)CU62} \)
7. \( \text{CU63(N G)CU64C40} \) 8. \( \text{FE54(N P)MN54} \)
9. \( \text{FE56(N P)MN56} \) 10. \( \text{I127(N 2N)I126} \)
11. \( \text{IN115(N N)115M} \) 12. \( \text{MG24(N P)NA24} \)
13. \( \text{MN55(N G)MN56C40} \) 14. \( \text{NA23(N G)NA24C40} \)
15. \( \text{NI58(N 2N)NI57} \) 16. \( \text{NI58(N P)CO58} \)
17. \( \text{NP237(N F)FP*B10} \) 18. \( \text{P31(N P)SI31} \)
19. \( \text{PU239(N F)FP*B10} \) 20. \( \text{S32(N P)P32} \)
21. \( \text{S34(N HE)SI31} \) 22. \( \text{SI28(N P)AL28} \)
23. \( \text{TH232(N F)FP*B10} \) 24. \( \text{TH232(N G)TH233} \)
25. \( \text{U235(N F)FP*B10} \) 26. \( \text{U238(N F)FP*B10} \)
27. \( \text{U238(N G)U239C40} \) 28. \( \text{ZN64(N P)CU64} \)
29. \( \text{ZR90(N 2N)ZR89} \)

It is necessary to submit the cross-sections every time to run the RDMM code. Thus, the author applied the CSTAPE program (a preceding program of SAND II code to generate the cross-section information and stored in the disk) to output the cross-section (in milli-barn) with range from 0.1 to 18 Mev in 0.1 Mev increments. The original cross-section range in CSTAPE program is separated into two regions, one by dividing from $10^{-10}$
to 1 Mev into 10 decades with 45 values in each decade, and the other by dividing the range from 1 to 18 Mev into 0.1 Mev increments.

Figures C.1 to C.4 and Table C are the cross-section information used in RDMM code.
Figure C.1. The cross-section as a function of neutron energy for $^{27}\text{Al}(n,\text{He})^{24}\text{Na}$, $^{27}\text{Al}(n,p)^{27}\text{Mg}$, $^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$. 
Figure C.2. The cross-section as a function of neutron energy for Fe54(n,p)Mn54, Fe56(n,p)Mn56, In115(n,n)In115m.
Figure C.3. The cross-section as a function of neutron energy for Au$^{197}$(n,γ)Au$^{198}$, Mg$^{24}$(n,p)Na$^{24}$, Ni$^{58}$(n,p)Co$^{58}$. 
Figure C.4. The cross-section as a function of neutron energy for Th232(n,f)FP, U235(n,f)FP, U238(n,f)FP.
Table C. Library Cross-section

1. For $\text{Al}_{27}(n,\text{He})\text{Na}_{24}$ as Energy 4.7(1.1)18

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2. For $\text{Al}_{27}(n,p)\text{Mg}_{27}$ as Energy 2.6(1.18)

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4. For Cu63(n,G)Cu64 as Energy $1.1(1.1)18$

| 5.751  | 5.672  | 5.593  | 5.514  | 5.435  | 5.356  |
| 5.277  | 5.198  | 5.119  | 5.040  | 4.973  | 4.918  |
| 4.863  | 4.808  | 4.753  | 4.698  | 4.674  | 4.588  |
| 4.533  | 4.478  | 4.429  | 4.386  | 4.344  | 4.301  |
| 4.010  | 3.981  | 3.951  | 3.922  | 3.892  | 3.863  |
| 3.833  | 3.804  | 3.774  | 3.745  | 3.718  | 3.694  |
| 3.670  | 3.646  | 3.622  | 3.598  | 3.574  | 3.550  |
| 3.070  | 3.058  | 3.046  | 3.034  | 3.022  | 3.010  |
| 2.998  | 2.986  | 2.974  | 2.962  | 2.950  | 2.938  |
| 2.926  | 2.914  | 2.902  | 2.890  | 2.878  | 2.866  |
\begin{align*}
&2.854 & 2.842 & 2.830 & 2.818 & 2.806 & 2.794 \\
&2.782 & 2.770 & 2.758 & 2.746 & 2.734 & 2.722 \\
&2.710 & 2.698 & 2.686 & 2.674 & 2.662 & 2.650 \\
&2.638 & 2.626 & 2.614 & 2.602 & 2.590 & 2.578 \\
&2.566 & 2.554 & 2.542 & 2.530 & 2.518 & 2.506 \\
&2.496 & 2.489 & 2.482 & 2.474 & 2.467 & 2.460 \\
&2.452 & 2.445 & 2.438 & 2.430 & 2.423 & 2.416 \\
&2.408 & 2.401 & 2.394 & 2.386 & 2.379 & 2.372 \\
&2.364 & 2.357 & 2.350 & 2.342 & 2.335 & 2.328 \\
&2.320 & 2.313 & 2.306 & 2.298 & 2.291 & 2.284 \\
\end{align*}

5. For Fe54(n,p)Mn54 as Energy \( .1(\cdot)18 \)
\begin{align*}
&.177 & .271 & .454 & .636 & .818 & 1.040 \\
&1.500 & 2.012 & 2.600 & 3.200 & 3.900 & 4.700 \\
&13.800 & 15.600 & 18.040 & 21.120 & 24.455 & 29.320 \\
&34.439 & 41.199 & 49.599 & 58.199 & 67.999 & 77.999 \\
&91.198 & 107.597 & 124.547 & 144.797 & 165.596 & 188.796 \\
&320.552 & 336.663 & 352.774 & 368.885 & 384.116 & 394.060 \\
&403.123 & 412.185 & 421.248 & 430.310 & 439.373 & 448.435 \\
&457.498 & 466.560 & 475.622 & 484.685 & 493.747 & 502.810 \\
&511.872 & 520.934 & 529.665 & 536.398 & 542.798 & 547.749 \\
&551.249 & 554.749 & 558.249 & 561.599 & 564.799 & 567.646 \\
&568.371 & 568.741 & 569.112 & 569.482 & 569.852 & 570.223 \\
&570.593 & 570.963 & 571.334 & 571.704 & 572.075 & 572.445 \\
&572.815 & 572.426 & 571.276 & 570.125 & 568.975 & 567.824 \\
\end{align*}
| 566.674 | 565.523 | 564.373 | 563.222 | 562.072 | 560.922 |
| 559.590 | 557.732 | 555.839 | 553.948 | 551.053 | 547.153 |
| 543.253 | 539.353 | 535.453 | 531.553 | 527.653 | 623.753 |
| 519.853 | 515.953 | 511.571 | 506.704 | 501.837 | 496.971 |
| 492.104 | 487.237 | 482.371 | 477.504 | 472.637 | 467.771 |
| 462.904 | 458.037 | 453.171 | 448.304 | 443.438 | 438.571 |
| 433.704 | 428.838 | 423.971 | 419.104 | 414.238 | 409.371 |
| 404.504 | 399.638 | 394.771 | 389.904 | 385.038 | 380.171 |
| 375.305 | 370.438 | 365.571 | 360.705 | 355.838 | 350.971 |
| 346.105 | 341.238 | 336.371 | 331.505 | 326.638 | 321.772 |
| 316.905 | 312.038 | 307.172 | 302.305 | 297.439 | 292.575 |
| 288.105 | 283.505 | 278.904 | 274.304 | 269.904 | 265.705 |
| 261.505 | 257.306 | 253.106 | 249.106 | 245.306 | 241.507 |
| 237.707 | 233.908 | 230.257 | 226.758 | 223.258 | 219.758 |
| 216.259 | 212.759 | 209.259 | 205.760 | 202.260 | 198.760 |

6. For Fe\(_56\)\((n,p)\)\(\text{ln}56\) as Energy \(3.6(\cdot1)18\)

| 0.002 | 0.007 | 0.017 | 0.032 | 0.046 | 0.059 |
| 0.067 | 0.072 | 0.118 | 0.206 | 0.300 | 0.400 |
| 0.525 | 0.675 | 0.922 | 1.267 | 1.825 | 2.595 |
| 3.510 | 4.570 | 5.800 | 7.200 | 8.699 | 10.299 |
| 32.120 | 33.117 | 35.419 | 37.939 | 40.459 | 42.979 |
| 45.297 | 46.400 | 47.300 | 48.200 | 49.100 | 50.087 |
| 51.599 | 53.199 | 54.799 | 56.399 | 58.024 | 59.799 |
7. For In$^{115}$(n,$n'$)In$^{115}$m as Energy \( E = 0.1 \) keV

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8. For Mg24(n,p)Na24 as Energy 5.1(.1)18

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9. For Ni58(n,p)Co58 as Energy 1.1(1)18

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11. For $U_{235}(n,f)FP$ as Energy $1(1.18$

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APPENDIX D

RECOMMENDATIONS IN USING COMPUTER CODES

In order to run the codes reliably and efficiently, several features are recommended as follows:

D.1 SAND II CODE

1. Name of foils must be the same as the short reaction name in library file. (see Appendix C)
2. Extrapolation forms
   LOW END E is suggested.
3. Auxiliary output
   NO PLOT NO CARDS is suggested.
4. For ITERATION RUN only
   LIMIT 25 and SMOOTH 1 are optimal values.

D.2 RDMM CODE

1. Number of foils no greater than 10.
2. Number of points in which the $\sigma(E)$ are tabulated NP = 180.
3. MIN = 3, MAX = 6 in most cases.
4. Number of Monte Carlo histories for each approximation order $NHIH(I) = 100$ for each I.
5. $E(1) = 0.1$, $H = 0.1$.
6. Scale factor, SCALE = 1.E19;
   Initial random digit, IX = 5.
D.3 SPECTRA CODE

1. Name of foils must be the same as the reaction name in library file. (see Appendix C)

2. Number of flux values in field 2 of input data 1 no greater than 35 is suggested.

3. Maximum number of iterations in field 5 of card 1, 1,000 - 2,000 are optional.

4. E(2)/E(1) value no greater than 10 is suggested.

5. It must be begun with heading card RUN, for every case, and ended with last card ENDEND for ceasing execution.
APPENDIX E

CURRENTLY OUTPUT DESCRIPTIONS

E.1 SAND II CODE

The first page is the data echo check.

In the next N+1 pages that follow the results of each iteration are listed, where N is the actually iteration numbers. These contain:

- Foil name, cover name, lower and upper 5% activity limits, measured to calculated activity ratio, and deviation (%) of measured from calculated activity. One line for one foil;
- Standard deviation (%) of measured activity;
- Average total flux (above 'NORM' Mev).

On the last page, an appropriate message is printed to indicate the reason for cessation of iteration, and the informations of saturated measured and calculated activity are added too.

The iteration process is currently stopped for any of the following occurs:

1. The standard deviation of measured-to-calculated activity ratios is smaller than the value specified on DEVIATION card;
2. The standard deviation becomes stable to within less than 1% in two successive iterations at a value higher than that specified;
3. The maximum allowed number of iterations (specified on LIMIT card) is reached.

In the next 17 pages that follow the detailed information is printed from energy range $10^{-10}$ to 18 Mev. (currently 621 intervals) These contain: energy value, absolute differential and integral flux value, normalized to 'NORM' Mev differential and integral flux value, and average energy value. One line for one energy value.

E.2 RDMM CODE

The first 5 or 6 pages contain:
- The title of the case;
- The coefficients $b_j$ of the functions $\psi_k$;
- The coefficient $w_k$ of the weighting function;
- The activity, its relative standard deviations and the cross-section relative standard deviations;
- The 'cut-off' numbers of the series expansion and the number of the Monte Carlo histories required;
- The scale factor;
- The elements of the matrices $S$ defined in formula (17);
- The elements of the matrices $R^T R$ defined in formula (22);

In the pages that follow the results of the
computation are listed. For each cut-off number 2 or 3 pages are printed. The first 1 or 2 pages contains:

- The elements of matrices $R^T R$ of that series expansion;
- The list of the numbers

$$\int_{A_i} \sigma_i \psi^k dE$$

- The value of the quadratic form $Q$ (see Eq. 20);
- The value of integral flux above 0.5 Mev;
- The table of the actual value of $\psi^k(E)$.

The next page is listed only if a statistical analysis on the results is required. This page contains all the information concerning this analysis on integral and differential neutron flux. This information is the total and mean flux value and their interval, calculated and Monte Carlo flux, absolute and relative standard deviation, and 68% confidence interval.

E.3 SPECTRA CODE

The first two or three pages:

- Input deck echo check;
- The names, activities and weight factors of the foils;
- Initial and normalized initial flux, initial and normalized initial calculated activity ratios;
- Elements of the matrix $C$ defined in Eq. 26;
- The results from subroutine LIMIT contain calculated differential and integral flux, calculated activities.

The next ten pages or more give the results from subroutine REPETE. This subroutine currently prints out the eigenvalues of $B^{-1}$, and the energy points first. It prints out results for each of the first 10 iterations, then every fifth iteration up to 100, then every 100th iteration. The results contain the calculated differential and integral flux values, the calculated activities, the calculated to measured activity ratios, the activity error, the root-mean-squared flux difference with respective to the trial.
APPENDIX F

CHARACTERISTICS OF THE UMR REACTOR

Type: Swimming Pool (modified BSR-type)
Core: Heterogeneous-uranium, aluminum, water
Al/H₂O Volume Ratio: 0.7 ± 0.05
Moderator: Light Water
Reflector: Light Water and Graphite
Coolant: Light Water with free convection flow
Biological Shield: Light Water and Normal Concrete
Critical Mass: 2.7 kg U-235 for Water Reflector
Power Level: Up to 200 Kw
Average Thermal Flux: $1.6 \times 10^{12}$ n/cm²-sec at 200 Kw with an H₂O reflector.

Tabulated results for differential flux operating at 200 Kw at core position 0.3 are listed in Table F.
The diagram of UMR Reactor core is shown in Figure F.1.
A key to the fuel prefixes is:

F - Standard Elements
C - Control Elements
S - Source Holder.
Figure F.1. Diagram of UMRR Core Loading 31T

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### Table F

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BIBLIOGRAPHY


VITA

Jau Wen Chen was born in Chunghua, Taiwan on November 3, 1944. He graduated from Taiwan Provincial Taichung First High School, Taichung, Taiwan, in July 1963.

October 1964, he entered National Tsing Hua University, Hsinchu, Taiwan. June 1968, he received a Bachelor of Science degree in Nuclear Engineering.

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