CHAPTER - 4

CROSS-SECTION ADJUSTMENT IN THE ANALYSIS OF SHIELDING BENCHMARK EXPERIMENTS

4.1 INTRODUCTION

Reactor Physics and Shielding calculations are limited in their accuracy by both computational methods and uncertainties in cross-section data. Refinements in calculational methods, particularly for deep penetration problems, were suggested in Chapter 2. This chapter deals with the errors in the cross-section data and their influence on the transport computations through thick shields. The procedure of cross-section adjustment is introduced for shielding calculations, in which differential measurements (cross-section data) and integral measurements are combined, with the help of sensitivity coefficients, to yield a data and method testing program.

Shielding calculations, including the estimates of uncertainties arising entirely from the input nuclear data, indicate that data caused uncertainties in the calculations are considerably greater than the errors claimed in the experiments [51-52]. This observation has opened up a new area in the field of shielding, known as data adjustments. In this approach, one
reaches into the data sets and with the help of sensitivities 'Adjust' the cross-sections to improve agreement with integral experiments. Such adjustment procedures have been practiced in the field of core physics [53]. However, the extension of the same method to the shielding domain becomes complicated since it is necessary to optimize the data sets to a large range of integral experiments, in addition to the constraints imposed by the uncertainties of both macroscopic and microscopic results.

The procedure employed in extending the sensitivity analysis to Data Adjustment is outlined below. In a subsequent section the development and testing of an adjustment code 'ADJUST' is discussed. Finally results of a test case are presented.

4.2 METHOD OF CROSS-SECTION ADJUSTMENT

The procedure is based upon the method of least squares. Let a physical quantity $x$ be normally distributed with a mean value $\bar{x}$ and a standard deviation $\Delta x$. Then the probability that a variable $x'$ will lie between $x'$ and $x' + dX$ is given by

$$ P(x')dx' \propto \exp \left\{ -\frac{1}{2} \left( \frac{x' - \bar{x}}{\Delta x} \right)^2 \right\} dx' $$
Let $Y$ be another quantity which is a function of $X$, $Y = Y(X)$ and whose measured values are normally distributed about $\bar{Y} = Y(\bar{X})$, with a deviation $\Delta Y$, then the probability density for obtaining $X', Y'$ in two independent measurements of $X$ and $Y$ is

$$P(X', Y')dX'dY' \propto \exp \left(-\frac{1}{2}\left[\left(\frac{X' - \bar{X}}{\Delta X}\right)^2 + \left(\frac{Y' - \bar{Y}}{\Delta Y}\right)^2\right]\right)$$

In practical cases, however $\bar{X}$, the 'true' value of $X$ is not known and the actual problem is to estimate its value from the results of measurements. When only $X$ is measured, one obviously concludes that $X = \hat{X} \pm \Delta \hat{X}$, where $\hat{X}$ and $\Delta \hat{X}$ denote the sample mean and sample variance respectively. But when $Y$ is also measured and one is given that $Y = \hat{Y} \pm \Delta \hat{Y}$, it is possible to improve the estimate of $\bar{X}$ with this additional information. The principle of Maximum likelihood [54] states that the best estimate of $\bar{X}$ is that value of $\bar{X}$ for which $P(X, Y)$ is maximum; or in other words,

$$Q = \left(\frac{\hat{X} - \bar{X}}{\Delta X}\right)^2 + \left(\frac{\hat{Y} - \bar{Y}}{\Delta Y}\right)^2$$

is a minimum. Let us apply this method to the data adjustment. Let $X = \{X_1, X_2, \ldots, X_N\}$ be a vector of the experimentally measured values. $g = \{g_1, g_2, \ldots, g_N\}$ be a vector of the calculated values. $g = g(p)$, that is $g$ is calculated from the cross-section set. $p = \{p_1, p_2, \ldots, p_L\}$ be a vector of the group cross-section and $Y$ be the initially given approximate cross-section set.
Then $Q$ may be written as

$$Q = \sum_j \frac{(X_j - g_j)^2}{\sigma_x^2} + \sum_k \frac{(p_k - Y_k)^2}{\sigma_y^2}$$

which should be a minimum. The above expression for $Q$ is true only if there are no correlations among the experimentally measured values.

With an ideal experimental set up, the individual measurements would be independent of each other. In reality, however, these measurements are far from being perfect. Due to factors such as systematic errors, normalization of relative measurements and interpolations etc., at least some (or even all) of the measured values are correlated. Of late experimentalists have become aware of these facts and try to find out the error covariance matrix for these measured values, if not to remove the factors which affect them \[55.65\].

In the absence of correlations, the covariance matrix will be just diagonal, whereas with this restraint, they give rise to off-diagonal elements.

Let $D_{ij} = \langle \delta X_i \delta X_j \rangle$ be the error covariance matrix of the measured values $X_i$ (i = 1, 2, ..., N) and $C_{kl} = \langle \delta Y_k \delta Y_l \rangle$ be the error covariance matrix of the measured cross-section set $Y(K = 1, 2, ..., L)$.

In this case,
Q becomes

\[ Q = \sum_{i,j=1}^{N} (X_i - g_i) D_{ij}^{-1} (X_j - g_j) + \sum_{k,l=1}^{L} (p_k - y_k) C_{k,l}^{-1} (p_l - y_l) \]

The expression for \( Q \) in the above equation may be written in matrix notation as

\[ Q = (X - g(p))^T D^{-1} (X - g(p)) + (p - y)^T C^{-1} (p - y) \quad \ldots \quad (4.1) \]

To minimise \( Q \), let us differentiate equation (4.1) and equate it to zero.

\[ \frac{\partial Q}{\partial p} = - (g' \cdot \frac{\partial p}{\partial p})^T D^{-1} (X - g) + C^{-1} (p - y) \]

\[ = - \left( \frac{\partial g}{\partial p} \right)^T D^{-1} (X - g) + C^{-1} (p - y) = 0 \quad (4.2) \]

The above equation can be solved by the linear approximation method where \( g(p) \) is expanded around \( Y \), and terms higher than linear are ignored, i.e.

\[ g(Y + \delta p) = g(Y) + \frac{\partial g}{\partial p} \delta p \]

Let \( p = Y + \delta p \); \( \delta p = (p - Y) \) and \( g_o = g(Y) \); \( \frac{\partial g}{\partial p} = S \), the matrix of sensitivity coefficients.

\[ g(p) = g_o + S(p - Y) \quad (4.3) \]

Using (4.3) in (4.2)
or

\[
\begin{align*}
& (S_D^{-1} S + C^{-1})(p - y) = S_D^{-1}(x - g_o) \\
& p = y + C^{-1}(p - y) \\
& p = p_o + P_o S_D^{-1}[x - g(p)]
\end{align*}
\]

where we have substituted \(p_o\) for \(y\) and \(P_o\) for \(C\).

Having found the value for \(p\), the adjusted group cross-section set, we need to consider the error in the calculation of \(p\).

To covariance matrix, \(p\) of the adjusted data set \(p\) is given by
\[ P = \langle \delta p \delta p^T \rangle \]

From equation (4.4)

\[ C^{-1}(p-y) = S^T D^{-1}[x - g(p)] \]

\[ C^{-1}(\delta p - \delta y) = S^T D^{-1}(\delta x - \delta g) \]

Using the relation \( S = \frac{\delta g}{\delta p} \) the above equation becomes

\[ C^{-1}(\delta p - \delta y) = S^T D^{-1}(\delta x - S \delta p) \]

Separating \( p \) terms,

\[ \left\{ C^{-1} + S^T D^{-1} S(p) \right\} \delta p = C^{-1} \delta y + S^T D^{-1} \delta x \]

Taking the direct product of LHS with itself we obtain the covariance matrix for the adjusted set as and obtaining ensemble average, we get the covariance matrix

\[ P(p) = \left\{ C^{-1} + S^T D^{-1} S(p) \right\}^{-1} \]

(4.5)

Here again we have to invert a matrix of the order of the number of parameters. Instead, we follow alternate approach using the iterative procedure.

Writing (4.5) as

\[ P(p) \left\{ C^{-1} + S^T D^{-1} S \right\} = I \]

\[ \left\{ P(p) C^{-1} + P(p) S^T D^{-1} S \right\} = I \]

\[ P(p) + P(p) S^T D^{-1} S C = C \]
or

\[ P(p) = C - P(p)S^{T}D^{-1}SC \]  

(4.6)

or

\[ P(p) = P_{o} - P(p)S^{T}D^{-1}SP_{o} \]  

(4.7)

where we have replaced \( C \) by \( P_{o} \).

Equations (4.4) and (4.7) solve iteratively for \( p \), adjusted cross-section set, and \( P \), the corresponding error associated with \( p \).

4.3 DEVELOPMENT OF THE ADJUSTMENT CODE

At the outset, it may be noted that the solutions of the equations (4.4) and (4.7) require the values of \( g \), \( S \) and \( X \). \( g \) and \( S \) are obtained as follows:

Let \( T(\tau) = T_{1}, T_{2}, \ldots, T_{N}(\tau) \) be the set of detectors, \( d\tau = dE dX \), the energy and space variables. Let \( \phi_{o}(p, \tau) \) be the flux distribution in the medium, evaluated using the cross-section set \( p \). Then the detector response

\[ g(p) = \int \phi_{o}(p, \tau) T(\tau) d\tau \]

\[ \frac{\partial g}{\partial p} = S = \int \frac{\partial \phi_{o}}{\partial p} T(\tau) d\tau \]

and \( S^{T} \), the transpose of \( S = \int \frac{\partial \phi_{o}}{\partial p} T(\tau) d\tau \)

Swanlake [67], one-dimensional perturbation code was chosen for the sensitivity calculations. However, the
code requires both the forward and the adjoint angular fluxes as input for the evaluation of sensitivity profiles. Discrete ordinate code ANISN [68] gives both the forward and adjoint angular fluxes. RADAK (PRC) [69-70] was used to obtain the response matrix of the detector.

4.3.1 Calculation of Forward and Adjoint Fluxes Using ANISN and Sensitivity Through S:\:\ANLAKE

ANISN [68] is a one-dimensional transport code written in FORTRAN IV. This uses the method of discrete ordinates to effect the numerical solution of the Boltzmann transport equation; the general theory of the $S_n$ method is described in ref.[71].

This section briefly describes the preliminary calculations performed using ANISN. Some tests were carried out with ANISN in order to establish a satisfactory mode of operation. The points considered in this connection were the energy group scheme and the order of the scattering expansion.

4.3.2 Cross-section Libraries

DLC-2 [42] was chosen for the data adjustment. ANISN accepts the cross-section in two different forms. In the normal mode, the cross-section data for all the groups and
elements are read and stored in the computer memory. Shielding calculations, however, require the use of large number of groups. In the present calculations, 100 group cross-section with 103 positions, 6 polynomials for each element were used (EURACOS-II benchmark experiment has three elements - C, Al and Fe). It may be noticed that they occupy a large amount of computer memory. This problem is overcome by using a group independent cross-section tape. In this case, ANISN keeps in the computer memory, only those cross-sections pertaining to the group it is processing. In other words, the code reads the cross-section group after group, thus reducing the computer memory to a large extent.

4.3.3 Adjoint Fluxes

ANISN solves the adjoint Boltzmann transport equation and yields the adjoint fluxes. The cross-section tables are to be transposed and energy reversed, so that in adjoint calculations the first group is the one having the less energy and the last group, the highest energy. This inversion of the cross-section data with respect to the group is done by the code only if they are fed in the normal way i.e. when all the cross-section values remain in the core of the memory. Such reversal is not done by the code if a group independent library is used. Therefore the code TAPEMA [72] was used to form the above group independent tapes (forward and adjoint) for the problem under consideration.
The fission spectrum was the input while calculating the forward fluxes. The detector responses form the source for the adjoint mode. As with the cross-section, all the adjoint sources must be supplied in the reversed group order (and in the reversed direction orders; - latter case was not applicable while dealing with the isotropic source).

4.3.4 **Calculation of Sensitivity Coefficients**

The one-dimensional perturbation programme SWANLAKE makes use of forward and adjoint calculations by ANISN to calculate the sensitivity coefficients. A brief description on the theory of sensitivity analysis is given in Chapter 1.

Sensitivity is defined as the fractional change in a reaction rate (resultant) \( f \) due to a given fractional change in an item of data \( X \) used by ANISN, i.e.

\[
U_i = \frac{\delta f}{f} \frac{\Delta X_i}{X_i}
\]

Here the group reaction cross-section pertaining to \( f \) are used as the source for the adjoint calculation.

The fractional change \( \delta X_i / X_i \) can apply to any of the partial cross-sections used by ANISN or to the total cross-section with all partial cross-sections increased by the same fraction.
Earlier we obtained the equation for $p$, adjusted group cross-section set, (see Eq. 4.4)

$$p = p_0 + P_0 S^T D^{-1} (X - g)$$

$$= p_0 + P_0 \int \frac{\delta \phi}{\delta p} T^T (\tau) D^{-1} (X - g) d$$

denoting

$$T^T (\tau) D^{-1} (X - g)$$ as $R^+$

$$p = p_0 + P_0 \int \frac{\delta \phi}{\delta p} R^+ (p, \tau) d \tau$$

where $R^+$ is the global detector as identified by McCracken [73]. Let

$$\int \frac{\delta \phi}{\delta p} R^+ (p, \tau) d \tau = F(p)$$

Then the above equation becomes

$$p = p_0 + P_0 F(p)$$

$F(p)$ is calculated from SWANLAKE as

$$F(p) = \int \frac{\delta \phi}{\delta p} R^+ (p, \tau) d \tau$$

Consider the transport equation $\Omega \phi = Q$ where $\Omega$ is the Boltzmann operator, $\phi$ the neutron flux and $Q$ the source.

Differentiating the above equation:

$$\frac{\delta \Omega}{\delta p} \phi + \Omega \frac{\delta \phi}{\delta p} = 0$$

$$\Omega \left( \frac{\delta \phi}{\delta p} \right) = - \frac{\delta \Omega}{\delta p} \phi$$
This may be interpreted as follows: \((\delta \Phi / \delta p)\) is a solution of the equation and the flux distribution is produced by the source \(- \frac{\delta \mathcal{O}}{\delta p} \cdot \Phi\).

Then we write

\[
F(p) = \int \frac{\delta \Phi}{\delta p} R^+(p, \tau) d\tau
= - \int \Phi^*_o(p, \tau) \frac{\delta \mathcal{O}}{\delta p} \Phi_o(p, \tau) d\tau
\]

Here \(\Phi^*_o\) is the adjoint flux produced by the source \(R^+\) (global detector).

The sensitivity profiles given by SWANLAKE are of the form

\[
V_{\gamma}(p) = \frac{\delta f / f}{\delta p / p}
\]

\(\gamma\) is the index for various parameters, viz., absorption, scattering, total etc., \(f\) the reaction rate or resultant. Data adjustment requires the parameter, \(\delta f / \delta p\)

\[
F_{\gamma}(p) = \frac{\delta f}{\delta p} = \frac{f(p)}{p} V_{\gamma}(p)
\]

4.3.5 Interpretation of Sensitivity Results

It may be pointed out that the results from the SWANLAKE code have to be analysed and properly interpreted before they are applied to the data adjustment. A discussion on this follows.
4.3.5.1 Choice of the adjoint source

As mentioned earlier, $R^+(p, \tau)$, the global detector, is the source for the adjoint run.

From the equation (4.4), we have

$$R^+(p, \tau) = T D^{-1}(X - g)$$

It may be seen that the adjoint source may be positive or negative depending upon whether $X$ is greater or smaller than $g$. Negative sources have no physical meaning and hence these cannot be fed into ANISN.

Positive and negative sources were therefore separated. ANISN was run twice in the adjoint mode, one for the positive source and another for the negative source, with the sign reversed. SWANLAKE calculations were done twice and the sensitivity coefficients obtained, say $F_1(p)$ and $F_2(p)$. The difference $F = F_1 - F_2$ gives the combined sensitivity coefficient for the problem. This was possible due to the linearity of the Boltzmann transport equation.

4.3.5.2 Distinguishing various quantities from SWANLAKE

SWANLAKE gives sensitivity profiles for:

i) Total cross-section, $F_T$

ii) Scattering cross-section, $F_S$

iii) Absorption cross-section, $F_A$. 
Scattering cross-section \( S \), available in the cross-section library is the sum of elastic and inelastic scattering i.e. \( S = \text{inelastic} + \text{elastic} = I + E \).

Defining \( X \) as the elastic and nonelastic cross-section \( X = I + A \), where \( A \) is the absorption cross-section, total cross-section is therefore given by:

\[
T = A + S \\
= A + I + E \\
= X + E .
\]

It has been realised that elastic and inelastic scattering cross-sections are to be adjusted separately [73]. For this SWANLAKE is run with the elastic scattering cross-section placed in the position of the total cross-section in the library. This gives the sensitivity profiles, \( F_E \) for the elastic component.

We then deduce the sensitivity coefficient, \( F_I \) for the inelastic scattering as:

\[
F_I = F_S - F_E .
\]

4.3.5.3 Calculation of the sensitivity in SWANLAKE for dependent parameters

Some parameters are measured directly and the others are derived from them. The latter are termed as dependent parameters. The following example will explain it further.
Let $T$, $A$, $X$, the total, absorption and the non-elastic be the independent parameters. The sensitivity profile is then given by

$$F = F(aT aA aX) = F_T \delta \sigma_T + F_A \delta \sigma_A + F_X \delta \sigma_X$$  \hspace{1cm} (4.9)

We assume further that we have supplied, $A$, $I$, and $E$ matrices for SWANLAKE.

With the definitions,

$$T = A + S = A + I + E = X + E; \text{ where } X = I + A$$

$$\sigma_A = \sigma_A$$

$$\sigma_I = \sigma_X - \sigma_A; \quad \sigma_E = \sigma_T - \sigma_X$$

and

$$\delta F = V_A \cdot \delta \sigma_A + V_I (\delta \sigma_X - \delta \sigma_A) + V_E (\delta \sigma_T - \delta \sigma_X)$$

$$= (V_A - V_I) \delta \sigma_A + (V_I - V_E) \delta \sigma_X + V_E \delta \sigma_T$$

\hspace{1cm} \cdots \hspace{1cm} (4.10)

Comparing the coefficients in equations (4.9) and (4.10)

$$F_A = (V_A - V_I)$$

$$F_X = (V_I - V_E)$$

$$F_T = V_E$$

\hspace{1cm} (4.11)

The same group independent tape prepared for ANISN cannot be used in SWANLAKE. The cross-section library has to be fed in the normal way. However, the computer
memory requirement for SWANLAKE are comparatively lower than those for ANISN. Hence there was no problem of storing the cross-section data in the computer memory.

4.3.5.4 Changes made in ANISN and SWANLAKE

The main program for the data adjustment should call ANISN and SWANLAKE in the iteration loop. These results in large amount of superfluous print out. In order to eliminate this, certain changes were made in these codes.

The quantities required from ANISN for the data adjustment are:

i) the total flux at various spatial mesh points.

ii) angular fluxes required for input to SWANLAKE.

The total flux are written by the code in FTO8 unit, and the angular fluxes normally go to FTO2, with FTO1 as an intermediate unit. In the adjoint mode, ANISN reuses both FTO1 and FTO2 units for the calculation of adjoint fluxes. The angular adjoint fluxes are finally written in FTO2 unit. Hence the angular fluxes from the forward ANISN run are to be transferred to some intermediate unit (FT15) before the ANISN is called for the adjoint run.

The total fluxes are also printed out by the code, which are the same as written in FTO8 unit. However, these are controlled by the subroutine WOT, which was made inactive for the purpose of data adjustment.
Similar changes were made in SWANLAKE, Subroutine WOT was made inactive. Additional units were introduced to obtain the required sensitivity matrix. FT17 unit gives the sensitivity of cross-section set by group and zone and the sensitivity of cross-section set summed over P(L) was written in FT18 unit.

Angular flux units, FTO1 and FTO2 were the same as in ANISN. FTO3 and FTO4 are the scratch units in SWANLAKE. These were changed to FT10 and FT11 to avoid conflicts with the code ANISN. Sensitivity matrix for the required cross-section set for various groups and positions are now available in FT11 unit.

The major portions of the code SWANLAKE contain plot subroutines. Though it is very useful to have such plots, they are of no great concern to the data adjustment. Hence all these subroutines were removed from the SWANLAKE.

4.3.6. The Code Adjust. The Main Program in the Data Adjustment

The computational procedure, featuring the important steps in the main program is given, below:

i) Set p = y
   .... Bench-mark loop

ii) Read Experimental values
iii) Calculate in the forward run
   a) the flux distribution $\phi_0(p, \tau)$
   b) the response $g(p)$
   c) the global detector, $R^+(p, \tau)$ or $R^-$ depending upon $x > g$

iv) Calculate the adjoint flux $\phi^*(p, \tau)$ with $R^+$ as the source

v) Calculate the sensitivity coefficients $F_1(p)$ and $F_2(p)$ using $\phi$ and $\phi^*$ from steps (ii) and (iii) and calculate $F = F_1 - F_2$ (see Section 4.3.5.1)

vi) Calculate the next approximation for $p$ and its correlation coefficient $P$ i.e. $p = p_0 + P F$

........ Benchmark loop ends.
Repeat the steps (ii) to (VI) till the convergence criterion on $p$ is achieved.

The code has been named ADJUST and the report gives full details of the input specifications and other relevant information [74]. All the modifications explained in section 4.3.5 were taken into account.

This section gives the potentialities of the code, ADJUST.

i) The data adjustment requires cross-section libraries in normal as well as in group independent forms. The procedures for obtaining them from one form to the other have been incorporated in it.
ii) Cross-section adjustments may be done only for some specified elements or for one or all the elements.

iii) The important feature of this code is simultaneously adjusting the cross-section from different benchmark experiments. The reader's attention is drawn to the position of the benchmark experiment loop inside the iteration loop. This has the following purpose.

We start with an assumption that the given group cross-section set is not the absolute one, but an approximate value. Every iteration improves the value of $p$. This is accomplished by making many measurements and adding them to the initial estimate. Thus:

$$\text{Initial estimate} + \text{Experiment} \rightarrow \text{New Estimate}$$

This may be interpreted as follows:

We try to understand more about the unknown parameter (in our case the group cross-section set $p$) with the help of additional experimental values and the sensitivity coefficients. Statistically, more the experimental values greater is the accuracy of $p$. In some cases, it may not be possible to get the desired number of experimental values or values with a desired accuracy. This may be due to some inherent difficulties in performing the benchmark experiments. This may be
overcome by getting the experimental values from other benchmark experiments.

Secondly, in analyzing more benchmark experiments, it will lead us to find out the systematic errors involved in the measurements, the goal with which we started with. The intrinsic errors arising from the instruments are difficult to eliminate, but they can be used to derive the covariance matrix for the initial values of the measured cross-section data. Correlations are minimized by repeating the experiments in various laboratories and in different conditions.

4.4 **BENCHMARK EXPERIMENTS**

The integral measurements required as one of the inputs are taken from the shielding benchmark experiments. These are conducted in ORNL [75] as well as in NEACRP [76]. Iron was chosen as the first material, because it is in widespread use in reactors. The aim of these experiments, was, among others, 'to investigate possible systematic errors and provide a test-bed for both experimental and analytical techniques, focussing attention on shielding studies, particularly deep penetration problems' [77].

We consider one benchmark experiment, EURACOS II [78-79] in this work. This facility is shown in Fig.4.1.
Fig. 4.1. Schematic diagram showing the benchmark facility of EURACOS
The neutrons from the core of the reactor pass through a thermal column (graphite). These thermal neutrons are incident on a converter plate producing fission neutrons. The converter plates are of trapezoidal shape and vary in size and form an almost a circular source of diameter, 80 cm. This is followed by an iron block of 137.7 cms thickness. The neutron flux in front of the centre of the source is of the order of $1 \times 10^9$ n/cm$^2$ [80]. A flux of this strength makes it possible to study neutron attenuation in a shield of upto a factor of about $10^5$ for fast neutrons and a factor of about $10^8$ for thermal neutrons. The spectral measurements using gas filled proportional counters and NE-213 organic liquid scintillators, were made at penetrations of 20.3, 50.8, 76.2 and 101.6 cms. In addition, activation foils such as $^{32}\text{S}(n,p)^{32}\text{P}$, $^{115}\text{In}(n,n')^{115}\text{In}$, $^{103}\text{Rh}(n,n')^{103}\text{Rh}$, $^{197}\text{Au}(n,r)^{198}\text{Au}$ and sandwich foil detectors of Au, W and Cu are also used. Although some off-axis measurements were performed, the analysis is concerned only with measurements along the central axis of the iron block.

Figures 4.2 through 4.4 show the spectra unfolded by RADAK [69] computer code, at the three measuring positions, viz. 50.8, 76.2 and 101.6 cms. The standard deviations on individual points indicated by the unfolding are not shown; the latter being less than 5%. Superimposed on the experimental spectra are fluxes calculated
FIG. 4.2. COMPARISON OF MEASURED AND CALCULATED SPECTRUM AT 50.8 cm PENETRATION IN IRON
FIG. 4.3 COMPARISON OF MEASURED AND CALCULATED SPECTRUM AT 76.2 cm PENETRATION IN IRON
FIG. 4.4. COMPARISON OF MEASURED AND CALCULATED SPECTRUM AT 101.6 cm PENETRATION IN IRON
with ANISN [68] and DOT [81] and Monte Carlo code, McNID [82]. The agreement with experiment is satisfactory at 50 cms. At 70 cms penetration the agreement of McNID calculation with experiment is better than that of DOT in the energy region of 30 keV to 300 keV. In the high energy region, i.e., above 800 keV, calculations are showing a tendency to underestimate the measured flux. This underestimate is even more marked at 101.6 cm where it reaches a factor of about 8 to 10 at 1 MeV [83]. Here it is relevant to find out the effect of impurities that are present in iron used in the experiment on the flux spectra. Table 4.1 shows the percentage of impurities in iron used in the EURACOS II. A new cross-section library, taking into account these impurities in iron was prepared. This was a 100 group cross-section data from the DLC-2 library. A comparison of the flux spectra at a depth of 100 cms for natural iron and iron with impurities is shown in Fig.4.5. It is seen that the impurities do not affect the results very much.

4.4.1 Results and Discussion

The integral measurements, corresponding to 50 cms depth in iron, were used and the code ADJUST was run. Adjustment factors were shown in Fig.4.6 for iron inelastic scattering cross-sections. Adjustment upto 25% has to be
Table 4.1 Percentage of Impurities in Iron used in EURACOS Benchmark Experiment

<table>
<thead>
<tr>
<th>Element</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn</td>
<td>0.600</td>
</tr>
<tr>
<td>Cu</td>
<td>0.390</td>
</tr>
<tr>
<td>Ni</td>
<td>0.135</td>
</tr>
<tr>
<td>Cr</td>
<td>0.130</td>
</tr>
<tr>
<td>C</td>
<td>0.130</td>
</tr>
<tr>
<td>Mo</td>
<td>0.024</td>
</tr>
<tr>
<td>Fe</td>
<td>98.591</td>
</tr>
</tbody>
</table>
FIG. 4.5. COMPARISON OF FLUX SPECTRA AT A DEPTH OF 100 cm
FOR NATURAL IRON AND THAT USED IN EURACOS
FIG. 4.6 INELASTIC CROSS SECTION
ADJUSTMENT FACTORS
made in this case. ANISN calculations were repeated with the adjusted cross-sections and compared with those of the experiments. There is an improved agreement at all energies at 50 cms (see Fig. 4.7) whereas the results at 101.6 cms (Fig. 4.8) are not that good, particularly at high energies. This discrepancy is due to the fact that only the experimental values at 50 cms were used for adjustment; it is necessary to include the measured values from all the distances for a better fit. Moreover, the error covariance used is that of Schmidt [58]. This gives information about the covariance between the total and all the partial cross-sections at a given energy. Correlations between values of cross-section at different energies were not used. In conclusion, we might say that we have gained confidence in achieving the aim of moving the calculated curve towards the experimental one.

4.5 CONCLUSIONS

It is clear that cross-section sensitivity analysis has become a routine part of the shield design process. The extensions of cross-section sensitivity studies to uncertainty analysis and data adjustments are probably inevitable developments and have proper places in the inventory of shielding tools. This stage of advancement has come to light at a time when there is a feeling that the work in the shielding area has come to its end.
FIG. 4.7. COMPARISON OF SPECTRAL DISTRIBUTION AFTER ADJUSTMENT OF CROSS SECTION DATA
(DEPTH 50.8 cm)
FIG. 4.8. COMPARISON OF SPECTRAL DISTRIBUTION AFTER ADJUSTMENT OF CROSS SECTION DATA (DEPTH 101.4 cm)
The accuracy of the cross-section data, on which all the rest of the superstructure is built, need not be overemphasised. Unfortunately, accurate measurements of the various cross-section types and for all the energies of interest seem to be impossible. Factors such as normalisation, interpolation, extrapolation etc. are therefore employed in determining the unknown parameters. Moreover, elastic or inelastic scattering cross-sections (depending upon the elements and energies) are normally deduced from other independent parameters. These parameters have proved to be the dominant reaction cross-sections. Also the uncertainties for these parameters are less accurately known. For example, nitrogen exhibits large uncertainties in the nonelastic cross-sections at higher energies (see ref.31, 32). The deep penetration calculations for neutrons in sodium-steel-iron (TSF benchmark, ORNL [84]) are at best accurate to within a factor of two to three, where 90% confidence limits are to be required. In the absence of higher accuracy differential cross-section data, only high quality integral measurements are needed to achieve the above design objectives. These considerations have naturally led us into the field of data adjustment.

There are arguments for and against the data adjustments. They stem from the following reasons:
i) The cross-section uncertainties, especially their correlations are high and largely unknown. Though only a few methods have been reported on their evaluation, their importance and necessities are never ignored. This task nevertheless calls for an active collaboration between 'good' experimentalists and 'good' theoreticians.

ii) More deep-lying difficulty in the justification given for the uncertainty analysis and particularly the cross-section adjustment is from the application of cross-section sensitivity. The sensitivities are problem dependent. Shielding calculations are in general far more sensitive to a far less accurate data field and small adjustments can have large effects on predicting shield performance. In other words, relatively moderate changes in the detector response, or in the source function or in the sequences and thicknesses of the shielding layers can result in a drastic difference in the cross-section sensitivities. It is unlikely that the set of integral measurements accessible to experiment can be so extensive as to cover the entire range of conditions encountered in the shield design. The detector responses in the shielding calculations include deposition, atomic displacements, helium production, biological dose and activation. The
integral experiments rarely mock-up even approximately more than a few of these detector responses and are never accessible to realistic measurements. To extrapolate conclusions from the restricted set of feasible integral experiments to all the design requirements is a risky business. Our understanding of the sensitivities at present, is limited; 'it is hard to explain why the cross-section sensitivities behave the way they do.' Furthermore, so far attempt is made to evaluate the sensitivities using only the first order perturbations. To what extent the higher order perturbations are going to effect the final results remains to be seen. Investigations on the sensitivity calculation with all the orders of perturbations using the Monte Carlo method are therefore undertaken. This is described in the next chapter.