CONF-740903-10

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# ESTIMATED DATA COVARIANCE FILES OF EVALUATED CROSS SECTIONS — EXAMPLES FOR $^{235}U$ AND $^{238}U$*

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## ABSTRACT

We review the status of development of formats and methods to represent uncertainty information of evaluated microscopic data in the ENDF/B system. Some examples of methods to obtain the data covariances of important cross sections for fertile and fissile nuclides are given. We give some examples of typical group cross sections covariance matrices obtained by processing the ENDF/B estimated data covariance files.

## I. INTRODUCTION

Most reactor transport calculations use evaluated nuclear data files for basic input data. It is often perceived that one of the major sources of uncertainties in the result of transport calculations, but certainly not the only one in many cases, is the uncertainty in the data used as input. One of the aims of transport sensitivity studies is to determine the uncertainties in the results of transport calculations due to data uncertainties. Many such studies have been done in the past for fast breeder reactors including the significant economic impacts of these uncertainties by Geeebler et al. (1), Barré et al. (2), Usachev et al. (3), Hummel et al. (4), and others. Since data uncertainty information was not available from the evaluated nuclear data libraries, the very large task of determining the covariance matrices had to be done by the authors of these studies who most often had not been involved in the evaluation process of the original data files. As a result many drastic and simplifying assumptions had to be made concerning the data uncertainties and their correlations. The authors of most such studies have often commented that such evaluation of the uncertainties in the data should be performed by the evaluators who are more familiar with the data base and that this information should be both easily available and unambiguous. The results of previous sensitivity studies would have greater credibility if the data uncertainties and their correlations had been handled in a more realistic fashion, although it is doubtful if the general conclusions would have been changed substantially, i.e. the data base used for fast breeder reactor design and analysis is not yet accurate enough for the needs. However, with the improvements in the data base and as we approach the targeted accuracies determined in these previous sensitivity studies, there is a

*Research sponsored by the U.S. Atomic Energy Commission under contract with Union Carbide Corporation.

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need for a better and more complete treatment of data uncertainties and correlations. In order to answer this need for ongoing sensitivity programs, the Cross Section Evaluation Working Group has started with ENDF/B-IV to introduce formats and methods to represent on the data tapes the estimated data covariances in the evaluated microscopic cross sections. These new files of the ENDF/B system can be processed, together with the cross section files, to generate the required group cross sections covariance matrices for sensitivity studies and other uses.

It is the purpose of this paper first to review briefly the status of development of formats and methods to represent estimated microscopic data covariance information in ENDF/B; second, to illustrate via a few examples ways in which the data covariance files may be generated for some fertile and fissile nuclide cross sections of interest in fast breeder programs; and third to show some example of typical group cross sections covariance matrices obtained by processing the files.

## II. THE ESTIMATED DATA COVARIANCE FILES OF ENDF/B-IV

Cross section data are represented in different ways on the ENDF/B tape. For a given nuclide in one file, denoted by MF = 2, is entered the information concerning resolved and unresolved resonance parameters, file MF = 3 contains integrated continuum cross sections as a function of energies, files MF = 4 and 5 are reserved for angular and energy distributions information respectively. A similar set of files denoted by MF values of 12, 13, 14 and 15 are reserved for gamma-ray production cross sections. The ENDF/B files attempt to represent to the best of our knowledge the basic microscopic data and as such are intended to be applications independent. Various unavoidable practical considerations however tend to make any given evaluation more useful or applicable to some particular applications. It is therefore all the more important to have appropriate "uncertainty files" built in the system to guide the users. If we are to preserve the aim of having application independent evaluations, it is essential that the uncertainty information entered in the files be for the quantities in the files. It is the burden of processing codes to generate from the basic microscopic information the required application dependent quantities of interest. Because a major format change, which would require major modifications to all processing codes presently using ENDF/B tapes as input, was not judged essential at this stage of development of the microscopic data covariance information, for data already formulated on the tape, separate files, i.e. new MF values, were allocated for this purpose. For new types of nuclear data, those not previously handled in the ENDF/B tapes, a more logical way of handling the evaluated microscopic quantities and their estimated covariances is being implemented. With ENDF/B-IV, due to the early stage of development of the system, the only type of covariance data being handled is for files MF = 3 and 13, i.e. the integrated cross sections as a function of energy. The covariance files have been assigned files MF = 33 and 43, obtained by adding 30 to the corresponding data files. For many, if not most, fast breeder applications it will be essential to have similar information for files MF = 2, 4 and 5, as well as 12, 14 and 15, to satisfy the needs and such extensions are being investigated.

In this paper we shall not go into the details of the formats and procedures developed (5), but only review the considerations employed for arriving

at these formats and concepts. It is generally understood that the evaluated microscopic nuclear data files in ENDF/B represent in some sense the "best estimates" or "most likely values" of these data at that time. For purposes of sensitivity studies the evaluations are interpreted to represent the probability distribution of an ensemble of a priori equally likely estimates of the true value of the data. The values of the data in the files give the most likely values of this distribution and the covariance files the covariances of this distribution. The distribution law is assumed to be the normal distribution law. The concept of the uncertainty in the result R of a transport calculation, which is a function of these data, is that it is related to the variance of this result obtained with the complete set of these equally likely estimates of the true data. In principle, if we build a system, we can then calculate the a priori uncertainty in a result R. However, once the system is built if we perform a measurement of this result R, with its estimated uncertainty, the total information content of our system has changed and, in principle we should be able to improve upon our knowledge of this distribution. This field of sensitivity studies, usually called cross sections adjustment, could also make use of the estimated data covariance information in the files.

In statistical language what we are dealing with are estimated joint probability distributions of any two evaluated microscopic cross sections in the library. Our problem is fully defined if we provide the covariances of the cross sections since we consider the distribution law to be normal and have identified the data in the cross section files with the expectation values of the distribution. Let $X_i$ and $Y_j$ stand for cross section type X and Y at energies $E_i$ snd $E_j$ respectively in one of the equally likely evaluations, then we need to deal with the quantities:

$$COV(X_i,Y_j) \equiv \langle (X_i - \overline{X}_i)(Y_i - \overline{Y}_i) \rangle \quad , \tag{1}$$

where $\overline{X}_i$ and $\overline{Y}_j$ are found in the cross section files, MF = 3, and the expectation value is taken over the ensemble of equally likely evaluations. Clearly at this stage of development for the ENDF/B system our major goal is only to provide a sizable improvement in the treatment of uncertainties at a cost which is commensurate with the expected gains. Due to the lack of general experience in the handling of such quantities for "evaluations" of any kind, we stand to learn rapidly much if we implement at first only a simple system, with possibly limited expansion capabilities, but with clearly the ability to handle some of the most serious deficiencies of previous treatments. The two major objectives were first to have a flexible treatment of the correlations between cross sections of the same or different types at different energies, and second to describe these covariances of the microscopic data on the tape, in such a manner that they can easily be processed to yield the required covariance matrices of group cross sections. The basic concept used in the formalism to achieve our aims is the expansion of the covariances of the energy dependent cross sections into elements which are fully correlated over a stated energy range. The covariance $COV(X_i,Y_j)$ is first expanded as a sum of components $COV^n(X_i,Y_j)$

$$COV(X_i,Y_j) = \sum_n COV^n(X_i,Y_j) \quad . \tag{2}$$

Each component $COV^n(X_i,Y_j)$ represents elements which are correlated over some energy range of X(E), and Y(E) as follows:

$$COV(X_i,Y_j) = \sum_n COV^n(X_i,Y_j) \quad . \tag{2}$$

Let the energy range of X(E) and Y(E) be broken up into nonoverlapping consecutive energy intervals, which we identify with the value of the lowest energy in each interval $E_k^n$, and associate with each energy interval an element $F_{xy,k}^n$, thereby creating an $(E_k^n, F_{xy,k}^n)$ table of values.

Let $S_i^k$ be an operator, where the subscript i refers to the energy $E_i$, and the superscript k refers to the $k^{th}$ interval of a table. This operator $S_i^k$ is defined to be unity when the energy $E_i$ is within the energy interval $E_k^n$ of the table and zero otherwise.

Depending upon the value of a flag associated with each such $(E_k^n, F_{xy,k}^n)$ table the following three types of covariance components are defined:

1) Absolute elements correlated only within each $E_k^n$ interval

$$COV^n(X_i,Y_j) \equiv \sum_k S_i^k S_j^k \, F_{xy,k}^n \quad , \tag{3}$$

2) Fractional elements correlated only within each $E_k^n$ interval

$$COV^n(X_i,Y_j) \equiv \sum_k S_i^k S_j^k \, F_{xy,k}^n \, \overline{X}_i \overline{Y}_j \quad , \tag{4}$$

3) Fractional elements correlated over all $E_k^n$ intervals

$$COV^n(X_i,Y_j) \equiv \sum_{k,k'} S_i^k S_j^{k'} \, F_{xy,k}^n \, F_{xy,k'}^n \, \overline{X}_i \overline{Y}_j \quad . \tag{5}$$

The complete formalism for ENDF/B-IV allows up to two such tables to be defined, according to the value of the flag, over the energy range of X(E) and Y(E) for each $COV^n(X_i,Y_j)$ component, thereby allowing other correlation patterns to be represented as well. Let us call the two tables $(E_k^n, F_{x,k}^n)$ and $(E_\ell^n, F_{y,\ell}^n)$ respectively then we also have:

4) Fractional elements correlated between the $E_k^n$ and $E_\ell^n$ intervals

$$COV^n(X_i,Y_j) = \sum_{k,\ell} S_i^k S_j \, F_{x,k}^n F_{y,\ell}^n \, \overline{X}_i \overline{Y}_j \quad . \tag{6}$$

Although a few other combinations are presently defined, they are only used to achieve a compact representation and only involve combinations of the above components. Future expansion of the system can easily be made by defining new combinations of the operators.

There are several advantages to this formalism:

1) It gives the covariance information about the microscopic cross sections in a compact form,

2) Group cross-section processing codes can easily be adapted to generate the covariance matrices of group cross sections. The introduction in the formalism of the operators $S_i^k$ guarantees that double integrals need not be performed, a proof we shall not give here. The computation reduces itself to very simple group cross section collapsing schemes using the various elements $F^n_{xy,k}$, or $F^n_{x,k}$ and $F^n_{y,\ell}$, as "weights." Already codes have been written to perform these calculations (6) and standard processing codes are being extended to routinely process the information (7).

3) Because it parallels very closely the method used by most experimentalists to analyze the estimated uncertainties in their data, it should facilitate greatly the preparation of these files in many instances.

## III. EXAMPLES OF ESTIMATED COVARIANCE MATRICES OF EVALUATED DATA

For ENDF/B-IV extensive estimated data covariance files have already been prepared for several nuclides: oxygen (8), nitrogen (8) and carbon (9). These preliminary files are presently being used (10) in order to determine the importance of a more complete treatment of the correlations in sensitivity studies. For fast breeder reactors it has long been established that the most sensitive cross sections for many parameters are the capture and fission cross sections of $^{235}U$, $^{238}U$ and $^{239}Pu$ and considerable data exist for these reactions (11). It is also known that correlations among these cross sections are important. We are currently in the process of generating appropriate files of estimated covariance matrices for a sensitivity program at ORNL (12). We shall now present some of the different methods we have investigated to determine the covariance matrices of these important cross sections. Our aim here is to indicate possible methods which could be used by evaluators to estimate these quantities in certain situations. We have for this purpose simplified somewhat the situation to better illustrate the methods. We strongly believe that, just as in the case of evaluating cross sections and possibly more so due to the lack of experience, the evaluation of the estimated covariances of the data will require considerable skill and judgement, may not be easily automated, and will very much benefit from extensive discussion with the feedback from various experts. It is in this spirit that we present our results.

Since we did not have yet the ENDF/B-IV evaluations for these nuclides, our preliminary work was done in the context of the ENDF/B-III set. Because our work was specifically to be used in fast reactor sensitivity studies, we aimed, in describing the microscopic data covariances, at obtaining plausible results for group structures which might reasonably be used in such studies. Because no adequate treatment of the resolved and unresolved resonance region exists yet in the system, we did not try at this stage to incorporate even crudely ways of taking into account selfshielding and Doppler effects. In fact, since the system is well adapted to the description of fine group structures, we decided to identify the covariances of the microscopic data with those of fine groups with infinite dilution. In a well designed system the final answers should not depend on the exact choice of the fine group structure. It is our intention in the files to be used in reactor sensitivity studies to go down to 0.1 lethargy units so as to

achieve this goal. In this initial study, since for historical reasons many experimentalists have also reported their data as averages over decimal groups, we treated for convenience the decimal averages as the microscopic data. We shall now report on three different cases that we have examined:

1. $^{235}U$ $\sigma(n,f)$ from 1 to 100 keV

These cross sections have been extensively studied in the last few years and four independent measurements using white neutron sources appear very consistent; they are those of Lemley et al. (13), Perez et al. (14), Gwin et al. (15) and Gaither et al. (16). The consistency of these data has been analyzed quantitatively by de Saussure and Perez (11) to be about 4% in magnitude and 2% in shape over this energy region. If we identify each one of these measurements with an independent assessment, or evaluation, of these cross sections, we may directly perform the operation indicated in Eq. (1) and take the averages over these four "equally likely determinations" of the cross sections. Using the numbers given in Table II of reference 11, the result we obtain is shown in Fig. 1. In this figure we have given the correlation matrix, COR(J,J), and the standard deviation, $\rho(I)$, in percent, rather than the covariance matrix COV(I,J). If we label by I and J the decimal groups, these are defined as:

$$\rho(I) \equiv \sqrt{COV(I,I)}/X(I) \quad , \tag{7}$$

with X(I) the group cross section in group I and,

$$COR(I,J) \equiv \frac{COV(I,J)}{\rho(I)\rho(J)} \quad . \tag{8}$$

It is evident that in this case, given such consistent data, indicating a good understanding of the experimental uncertainties and methods, alternate ways of generating the covariance matrix could be used.

2. $^{238}U$ $\sigma(n,\gamma)$ from 1 to 100 keV

The data situation here is more complex than for $^{235}U$ (for a review of it, see reference 11). Basically the three recent time-of-flight white source measurements by Moxon (17), de Saussure et al. (18) and Fricke et al. (19) are not consistent. Because of considerable fluctuations in this cross section as a function of energy, the quasi-monoenergetic measurements do not provide much assistance. For ENDF/B-III, since the shapes of two of these measurements (ref. 17 and 18) were similar, it was mostly used in the evaluation, but the normalization was based on the average value of several quasi-monoenergetic measurements about 30 keV. Because the analysis of the measurements has failed to provide an understanding of the sources of the discrepancies, an empirical method of determining the covariances must be used. Because the ENDF/B-III curve represented the best understanding of all these data, it seems justified to use it to represent the average values in relation (1) but to perform the operations indicated using all three sets as equally likely values. The result of this procedure is indicated in Fig. 2 where again we have presented the correlation matrix for the decimal group and the standard deviations. This empirical method, although somewhat arbitrary, appears to yield plausible results which reflect the present status of our lack of adequate knowledge of these cross sections.

### 3. $^{238}U$ $\sigma(n,\gamma)$ from .1 to 10 MeV

We choose this example because it is fairly different from the two previous ones. The data situation is again reviewed in reference 11. We do not have as before a series of measurements which all span the complete energy range; rather the measurements are sparse and even with some gaps left unmeasured. Instead of trying to obtain the covariance matrix from the data base, we found that there were four other evaluations, besides ENDF/B-III, which were apparently independently performed, used almost the same data base, but yet gave rather different results. These are those of Davey (20), Sowerby et al. (21), Abagyan et al. (22) and Woll (23). We assumed that the four above evaluations were equivalent and equally likely, the differences being due to different "understanding" of the data base. We determined the infinitely dilute group cross sections for decimal intervals for these evaluations and applied the procedure given in Eq. (1); the result is shown in Fig. 3. The remarkable point of Fig. 3 is that the uncertainty given by our method is considerably higher than estimated by the evaluators themselves. As a comment on this point we will quote from reference 11: "Sowerby et al. (21) estimate that the U-238 capture cross section is known to 7% from .1 to 1 MeV; in the same range ENDF/B-IV (24) estimates an uncertainty of 5%. We think that these estimates are very optimistic, considering that there is more than 20% discrepancy around 1 MeV between the 1973 evaluation of Sowerby et al. and ENDF/B-IV!"

## IV. THE PROCESSING OF COVARIANCE FILES

The covariances of the U-238 capture cross sections in the range of 1 keV to 10 MeV generated as explained in the previous section were represented in the ENDF/B-IV format in exactly the details shown on Figs. 2 and 3. A processing code was written (6) to generate covariance matrices of group cross sections using the ENDF/B-IV files as input. This code was used to generate covariance matrices of group cross sections for a group structure typical of those used in fast reactor design and analysis. The particular group structure used was patterned after the 26 groups ABN set truncated at 1 keV and 10 MeV (referred to as MNG groups). Two different weighting schemes were used: $1/E$ and $1/E\sigma_T$, but infinite dilution was used in both cases. The results shown in Figs. 4 and 5 clearly indicate the type of structure to be expected in the correlation matrix from a more realistic handling of the covariances of the data, which is now possible with the ENDF/B system. Several comments should be made regarding the results shown on the figures:

1) The complete lack of correlation between the low and high energy groups, at 100 keV, is very unrealistic in its sharpness and is due to the lack of efforts made in our example in properly treating the transition region.

2) The differences between the two covariance matrices are completely negligible in view of the large uncertainties in the values of the elements. In the low energy region the similarity is also in large part due to the complete neglect of the resonance structure in our examples. The correlation between $\sigma_T$ and $\sigma_{n,\gamma}$ should strongly affect the matrix elements if

properly taken into account. Extension of the formalism to treat the resonance regions should remove this deficiency.

3) The computation of the covariance matrices, once the group cross sections were obtained took less than two seconds of PDP-10 CPU time, a very acceptable price paid for the flexibility of the system.

## V. CONCLUSIONS

In this paper we have shown that at least for continuum cross sections the system developed for ENDF/B to handle the covariances of the microscopic data is capable of representing a fair amount of details in a workable manner, and that this information can be processed easily to obtain the covariance matrix of multigroup cross sections needed in sensitivity studies. We have also shown by means of three simple examples covering rather different situations ways of obtaining plausible covariance matrices of the microscopic cross sections. Although we have not given any examples, the methods outlined may be used to obtain the covariances of any two different cross sections, either in the same or different nuclides, if ratio measurements are available. Since covariance matrices generated within the system outlined in this paper have not yet been used in sensitivity studies, it is not clear that large effects will be found in sensitivity studies results, compared to previous methods, but it is evident that these results will be more credible. Finally, we must note that much work remains to be done within the system to accommodate the special problems of the resolved and unresolved resonance regions.

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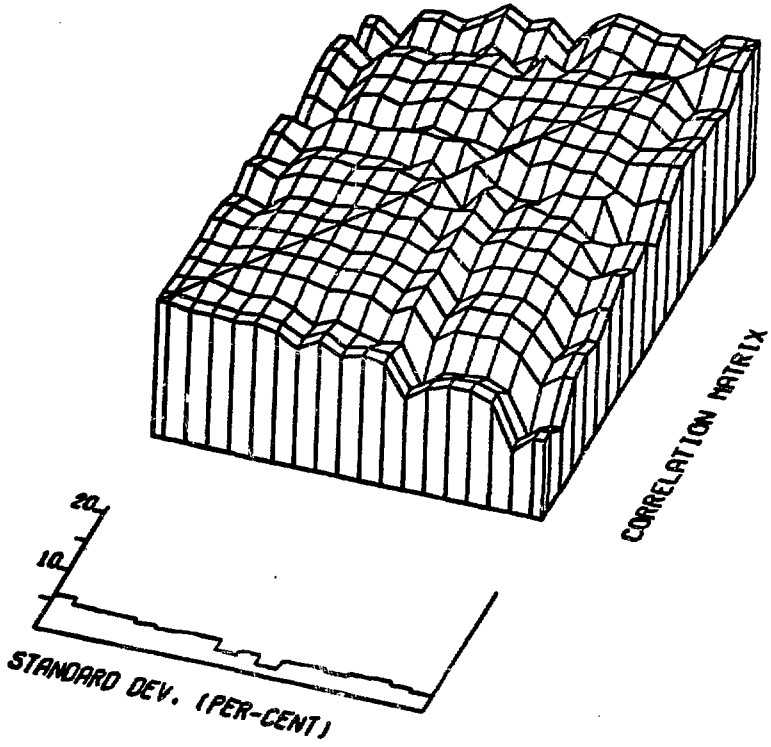
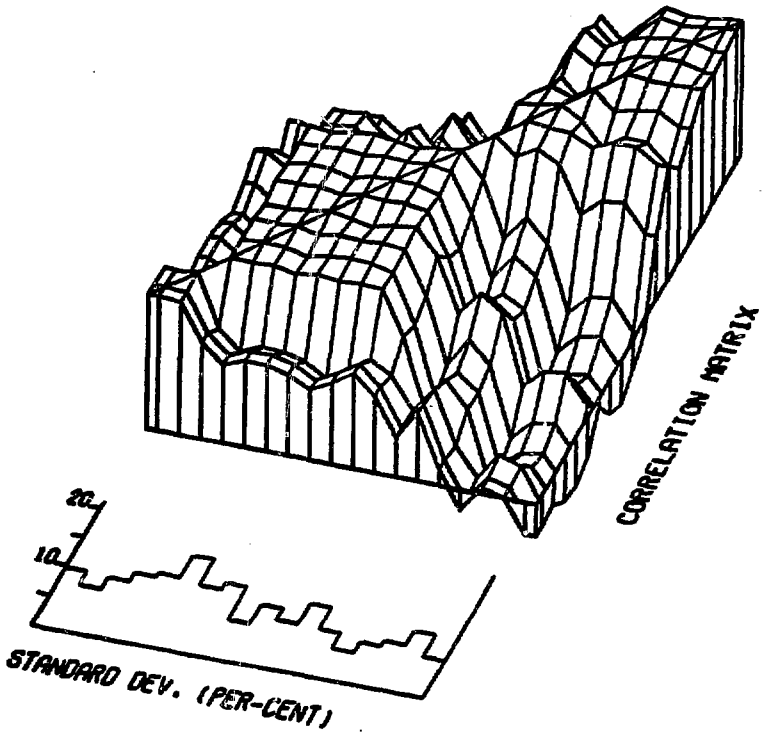
ORNL-DWG 74-8156



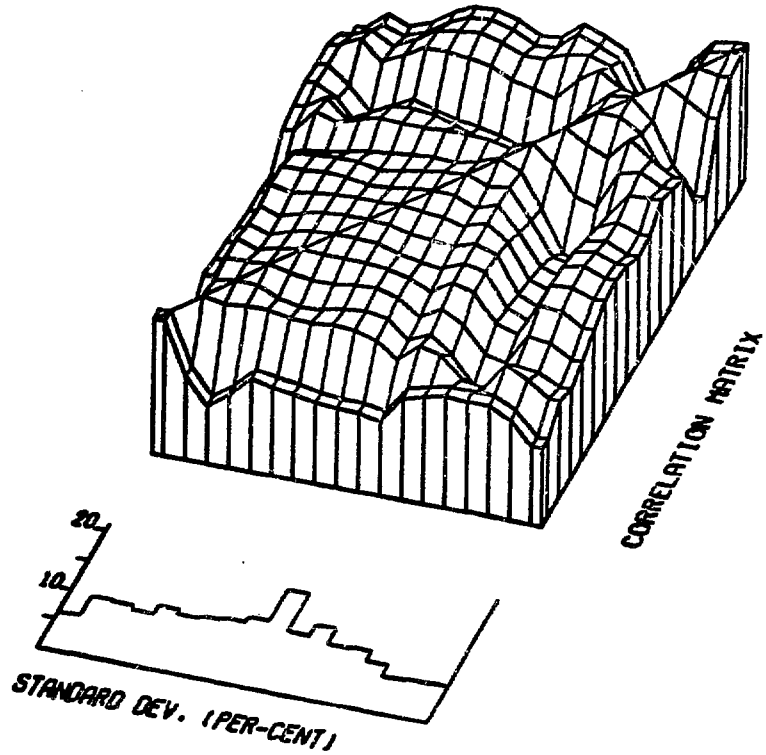

U-235 FISSION (DEC. GROUPS 1-100 KEV)

ORNL-DWG 74-8152




U-238 CAPTURE (DEC. GROUPS 1-100 KEV)

ORNL-DWG 74-8151

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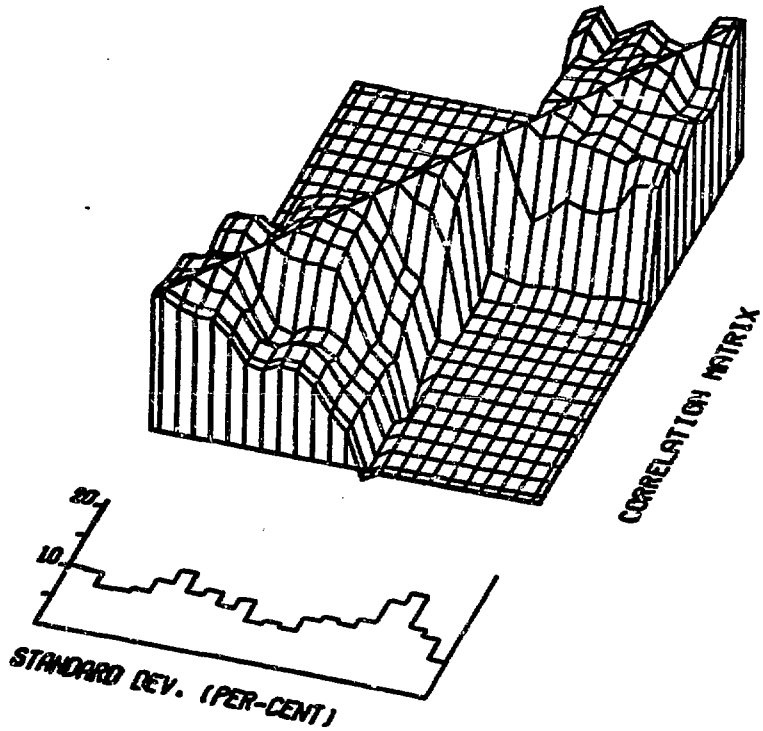
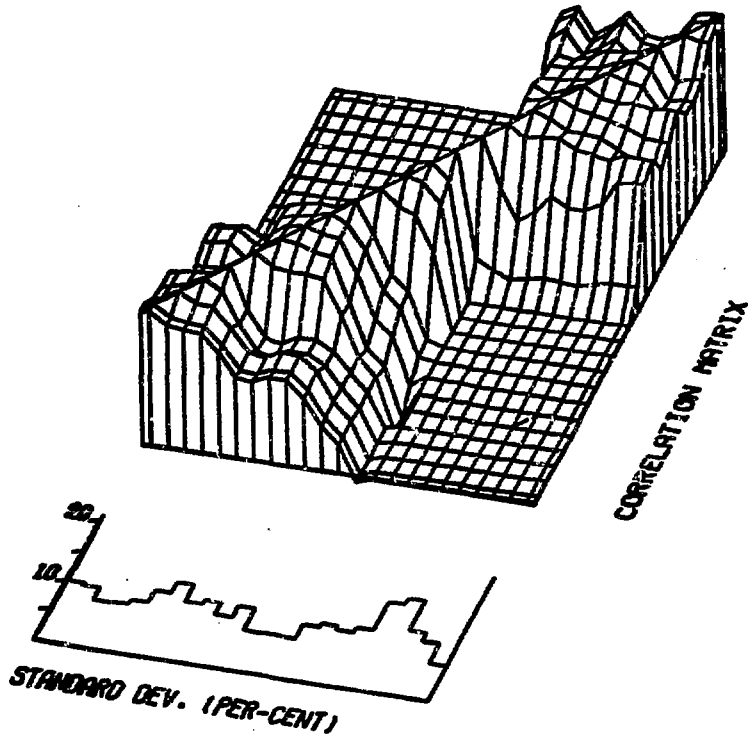
ORNL-DWG 74-8154




U-238 CAPTURE (MNG GROUPS.1/ESIGT-WEIGHTING)

ORNL-DWG 74-8153




U-238 CAPTURE (MNG GROUPS, E-WEIGHTING)