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DBUFIT - I

A LEAST SQUARES ANALYSIS CODE
FOR NUCLEAR BURNUP DATA

R. P. Matsen

May 1970

AEC RESEARCH & DEVELOPMENT REPORT

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DBUFIT - I
A LEAST SQUARES ANALYSIS CODE FOR NUCLEAR BURNW DATA

By

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May 1970

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ABSTRACT

The computer code, DBUFIT-I, is designed to extract integral cross section information from isotopic burnup data. This information is obtained by fitting burnup equations to the isotopic data using least squares fitting techniques. The burnup equations applicable to plutonium and uranium-plutonium fuels are described. The application of the code is illustrated by a sample burnup problem.

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INTRODUCTION

Knowledge of reaction cross sections is fundamental for an accurate description of the isotopic transmutations that occur during the irradiation of nuclear fuels. Integral values for these reaction cross sections (defined to be the spectral averaged cross section over the neutron energy range 0 to 10^8 eV) are important for the verification of analytical methods commonly used in the design of nuclear reactors. A computer code called DBUFIT-I has been developed for obtaining this type of integral cross section information from isotopic burnup data. The DBUFIT-I code (a double precision burnup fitting code - version I) obtains this information by fitting transmutation equations that describe the burnup process, to the isotopic data. The parameters of the least squares fit are ratios of these integral or flux averaged cross sections (hereafter simply referred to as cross section ratios). The code is written in FORTRAN V for use on the UNIVAC 1108 computer and is an adaptation of the more general least squares code, LIKELY,⁽¹⁾ The DBUFIT-I code is an improvement over the DUBLIK⁽²⁾ code which was previously used for the least squares analysis of burnup data.

The characteristics and use of the DBUFIT-I code are described in the following three sections. The differential and integrated burnup equations for plutonium and uranium-plutonium fuels are presented first. Next, the way in which the DBUFIT-I code has been adapted from the LIKELY code is explained. This section can be omitted by readers who are primarily interested in the application of the code to burnup problems since it has been written for those readers who are familiar with the concepts embodied in the LIKELY code and wish to understand the changes that have been made. The next section is basically a user's guide to the DBUFIT-I code which includes a sample burnup

problem as an example of the proper use of the code and the interpretation of its results. Additional items which bear on the successful application of the DBUFIT-I code to burnup data are also discussed in this section. The final section discusses several proposed improvements to the DBUFIT-I code.

FORMULATION OF THE INTEGRAL BURNUP EQUATIONS

Burnup equations have been previously presented,⁽³⁾⁽⁴⁾ which describe the major transmutations occurring in both plutonium and uranium-plutonium fueled reactor systems.

PLUTONIUM SYSTEMS

For a plutonium system the differential transmutation equations are:⁽³⁾

²³⁹Pu:

$$\frac{dN^{49}}{dt} = -\hat{\sigma}_a^{49} N^{49} \phi$$

$$\frac{dN^{49}}{dt} = -\hat{\sigma}_a^{49} N^{49} \phi$$

²⁴⁰Pu:

$$\frac{dN^{40}}{dt} = \hat{\sigma}_c^{49} N^{49} \phi - \hat{\sigma}_a^{40} N^{40} \phi$$

$$\frac{dN^{40}}{dN^{49}} = -\frac{\hat{\sigma}_c^{49}}{\hat{\sigma}_a^{49}} + \frac{\hat{\sigma}_a^{40}}{\hat{\sigma}_a^{49}} \frac{N^{40}}{N^{49}}$$

²⁴¹Pu:

$$\frac{dN^{41}}{dt} = \hat{\sigma}_a^{40} N^{40} \phi - \hat{\sigma}_a^{41} N^{41} \phi - \lambda^{41} N^{41}$$

$$\frac{dN^{41}}{dN^{49}} = -\frac{\hat{\sigma}_a^{40}}{\hat{\sigma}_a^{49}} \frac{N^{40}}{N^{49}} + \frac{\hat{\sigma}_a^{41}}{\hat{\sigma}_a^{49}} \left(1 + \frac{\lambda^{41}}{\hat{\sigma}_a^{41} \phi} \right) \frac{N^{41}}{N^{49}}$$

²⁴²Pu:

$$\frac{dN^{42}}{dt} = \hat{\sigma}_c^{41} N^{41} \phi - \hat{\sigma}_a^{42} N^{42} \phi$$

$$\frac{dN^{42}}{dN^{49}} = -\frac{\hat{\sigma}_c^{41}}{\hat{\sigma}_a^{49}} \frac{N^{41}}{N^{49}} + \frac{\hat{\sigma}_a^{42}}{\hat{\sigma}_a^{49}} \frac{N^{42}}{N^{49}}$$

²⁴³Am:

$$\frac{dN^{53}}{dt} = \hat{\sigma}_a^{42} N^{42} \phi - \hat{\sigma}_a^{53} N^{53} \phi$$

$$\frac{dN^{53}}{dN^{49}} = -\frac{\hat{\sigma}_a^{42}}{\hat{\sigma}_a^{49}} \frac{N^{42}}{N^{49}} + \frac{\hat{\sigma}_a^{53}}{\hat{\sigma}_a^{49}} \frac{N^{53}}{N^{49}}$$

^{244}Cm :

$$\frac{dN^{64}}{dt} = \hat{\sigma}_a^{53} N^{53} \phi - \hat{\sigma}_a^{64} N^{64} \phi - \lambda^{64} N^{64} \quad \frac{dN^{64}}{dN^{49}} = - \frac{\hat{\sigma}_a^{53}}{\hat{\sigma}_a^{49}} \frac{N^{53}}{N^{49}} + \frac{\hat{\sigma}_a^{64}}{\hat{\sigma}_a^{49}} \left(1 + \frac{\lambda^{64}}{\hat{\sigma}_a^{64} \phi} \right) \frac{N^{64}}{N^{49}}$$

where the superscripts designate the various isotopes (e.g., $49 = ^{239}_{94}\text{Pu}$, $40 = ^{240}_{94}\text{Pu}$, ..., $53 = ^{243}_{95}\text{Am}$, etc.), $N^{\mathbf{i}}$ is the isotopic concentration (in say atoms/barn-cm or atoms/original gram of plutonium) of the $\mathbf{i}^{\text{th}}$ isotope, $\lambda^{\mathbf{i}}$ is the decay constant for the $\mathbf{i}^{\text{th}}$ isotope (the $\lambda^{\mathbf{i}}$ for isotopes other than $^{241}_{94}\text{Pu}$ and $^{244}_{96}\text{Cm}$ are negligibly small), and t is the time variable. The quantity

$$\hat{\sigma}_j^{\mathbf{i}} = \frac{\int \sigma_j^{\mathbf{i}}(E) \phi(E) dE}{\phi}$$

where

$$\phi = \int \phi(E) dE$$

is the flux-averaged integral cross section for the $\mathbf{i}^{\text{th}}$ isotope (the subscripts are $j = a$ for absorption and $j = c$ for capture).

The equations in the second column were obtained by dividing the equations of the first column by dN^{49}/dt . The advantage of this transformation is that the unmeasured flux-time variable is eliminated from all but the first equation. The equations other than this first one involve only isotopic concentrations (which can be accurately measured) and ratios of the flux-averaged cross sections. The fact that the cross sections now appear in ratios rather than individually is a result of the process that removed the flux-time variable from the analysis.

Assuming that the cross section ratios are of the simple form

$$\hat{\sigma}_c^{49}/\hat{\sigma}_a^{49} = \epsilon, \quad \hat{\sigma}_a^{40}/\hat{\sigma}_a^{49} = A + AA/N^{40}, \quad (\hat{\sigma}_a^{41}/\hat{\sigma}_a^{49})(1 + \lambda^{41}/\hat{\sigma}_a^{41} \phi) = B$$

$$(\hat{\sigma}_c^{41}/\hat{\sigma}_a^{49})/(1 + \lambda^{41}/\hat{\sigma}_a^{41} \phi) = \gamma \quad \hat{\sigma}_a^{42}/\hat{\sigma}_a^{49} = C, \quad \hat{\sigma}_a^{53}/\hat{\sigma}_a^{49} = D, \text{ and}$$

$$(\hat{\sigma}_a^{64}/\hat{\sigma}_a^{49})(1 + \lambda^{64}/\hat{\sigma}_a^{64} \phi) = E$$

the solution to the set of differential burnup equations in the right hand column is

$$1. \quad N^{40} + AA/A + \frac{E}{1-A} N^{49} - K_0 (N^{49})^A = 0$$

$$2. \quad N^{41} - \frac{\varepsilon A}{(1-A)(1-B)} N^{49} + \frac{AK_0}{A-B} (N^{49})^A - K_1 (N^{49})^B = 0$$

$$3. \quad N^{42} + \frac{\gamma \varepsilon AB}{(1-A)(1-B)(1-C)} N^{49} - \frac{\gamma ABK_0}{(A-B)(A-C)} (N^{49})^A + \frac{\gamma BK_1}{B-C} (N^{49})^B - K_2 (N^{49})^C = 0$$

$$4. \quad N^{53} - \frac{\gamma \varepsilon ABC}{(1-A)(1-B)(1-C)(1-D)} N^{49} + \frac{\gamma ABCK_0}{(A-B)(A-C)(A-D)} (N^{49})^A - \frac{\gamma BCK_1}{(B-C)(B-D)} (N^{49})^B \\ + \frac{CK_2}{C-D} (N^{49})^C - K_3 (N^{49})^D = 0$$

$$5. \quad N^{64} + \frac{\gamma \varepsilon ABCD}{(1-A)(1-B)(1-C)(1-D)(1-E)} N^{49} - \frac{\gamma ABCDK_0}{(A-B)(A-C)(A-D)(A-E)} (N^{49})^A \\ + \frac{\gamma ABCD}{(B-C)(B-D)(B-E)} (N^{49})^B - \frac{CDK_2}{(C-D)(C-E)} (N^{49})^C + \frac{DK_3}{D-E} (N^{49})^D - K_4 (N^{49})^E = 0$$

where the K_i are constants of integration. The value of K_1 depends upon the adjustable parameters of its fitting equation which are (a) the cross section ratios (i.e., A, B, ε , etc.) and (b) the isotopic concentration of the i^{th} isotope measured at a given ^{239}Pu concentration. In the case of the DBUFIT-I code, the K_i are evaluated using the ^{239}Pu concentration of the first data point. There is also an option within the code that forces the fit through the first data point, if desired. In this case the fitting parameters consist solely of the

cross section ratios. In summary, the integrated equations are relationships between the measured isotopic concentrations and a set of parameters representing (a) the cross section ratios and (b) the initial concentrations while excluding the unmeasured flux time variable. Under the rather restrictive form assumed for the cross section ratios, these equations analytically describe the burnup path in isotopic concentration space,

The decay term $\lambda^{41}/\sigma_a^{41} \phi$ is small (generally $0.02 \leq \lambda^{41}/\sigma_a^{41} \phi \leq 0.10$ and is therefore treated as a corrective term rather than as one of the fitting parameters. It can be evaluated for each data point from the relationship

$$\lambda^{41}/\sigma_a^{41} \phi = \frac{\lambda^{41} \Delta t}{(\hat{\sigma}_a^{41}/\hat{\sigma}_a^{49}) \ln(N_O^{49}/N^{49})}$$

derived from $N^{49} = N_O^{49} e^{-\sigma_a^{49} \phi \Delta t}$ which is the integrated form of the first differential burnup equation. The zero subscript on N_O^{49} denotes the initial value for that isotope and Δt is the time interval during which the fuel was irradiated. Once $\lambda^{41}/\sigma_a^{41} \phi$ has been determined for each data point, a mean value and one standard deviation error is assigned to it and applied to all of the data used in the burnup analysis.

The fractional depletion of plutonium, β , can be calculated after the least squares parameters have been determined. Excluding a negligible contribution from ^{242}Pu neutron capture, β is the sum of the ^{239}Pu and ^{241}Pu atoms destroyed divided by the initial plutonium concentration.

$$\beta = \frac{(N_O^{49} - N^{49})(1-\epsilon) + (N^{42} - N_O^{42})(1-\gamma)/\gamma}{N_O^{49} + N_O^{40} + N_O^{41} + N_O^{42}}$$

where the zero subscript denotes an initial value.

URANIUM-PLUTONIUM SYSTEMS

The differential equations **which** describe the transmutation of a uranium-plutonium system are: (4)

^{235}U :

$$\frac{dN^{25}}{dt} = - \hat{\sigma}_a^{25} N^{25} \phi$$

$$\frac{dN^{25}}{dt} = - \hat{\sigma}_a^{25} N^{25} \phi$$

^{238}U :

$$\frac{dN^{28}}{dt} = - \hat{\sigma}_a^{28} N^{28} \phi$$

$$\frac{dN^{28}}{dN^{25}} = \frac{\hat{\sigma}_a^{28} N^{28}}{\hat{\sigma}_a^{25} N^{25}}$$

^{236}U :

$$\frac{dN^{26}}{dt} = \hat{\sigma}_c^{25} N^{25} \phi - \hat{\sigma}_a^{26} N^{26} \phi$$

$$\frac{dN^{26}}{dN^{25}} = - \frac{\hat{\sigma}_c^{25}}{\hat{\sigma}_a^{25}} + \frac{\hat{\sigma}_a^{26} N^{26}}{\hat{\sigma}_a^{25} N^{25}}$$

^{237}Np :

$$\frac{dN^{37}}{dt} = \hat{\sigma}_{n,2n}^{28} N^{28} \phi + \hat{\sigma}_a^{26} N^{26} \phi - \hat{\sigma}_a^{37} N^{37} \phi$$

$$\frac{dN^{37}}{dN^{25}} = - \frac{\hat{\sigma}_{n,2n}^{28} N^{28}}{\hat{\sigma}_a^{25} N^{25}} - \frac{\hat{\sigma}_a^{26} N^{26}}{\hat{\sigma}_a^{25} N^{25}} + \frac{\hat{\sigma}_a^{37} N^{37}}{\hat{\sigma}_a^{25} N^{25}}$$

^{238}Pu :

$$\frac{dN^{48}}{dt} = \hat{\sigma}_a^{37} N^{37} \phi - \hat{\sigma}_a^{48} N^{48} \phi$$

$$\frac{dN^{48}}{dN^{25}} = - \frac{\hat{\sigma}_a^{37} N^{37}}{\hat{\sigma}_a^{25} N^{25}} + \frac{\hat{\sigma}_a^{48} N^{48}}{\hat{\sigma}_a^{25} N^{25}}$$

^{236}Pu :

$$\frac{dN^{46}}{dt} = \frac{1}{2} \hat{\sigma}_{n,2n}^{37} N^{37} \phi - \hat{\sigma}_a^{46} N^{46} \phi - \lambda^{46} N^{46}$$

$$\frac{dN^{46}}{dN^{25}} = - \frac{1}{2} \frac{\hat{\sigma}_{n,2n}^{37} N^{37}}{\hat{\sigma}_a^{25} N^{25}} + \frac{\hat{\sigma}_a^{46} N^{46}}{\hat{\sigma}_a^{25} N^{25}} - \left(1 + \frac{\lambda^{46}}{\hat{\sigma}_a^{46} \phi}\right) \frac{N^{46}}{N^{25}}$$

^{239}Pu :

$$\frac{dN^{49}}{dt} = \hat{\sigma}_c^{28} N^{28} \phi - \hat{\sigma}_a^{49} N^{49} \phi$$

$$\frac{dN^{49}}{dN^{25}} = - \frac{\hat{\sigma}_c^{28} N^{28}}{\hat{\sigma}_a^{25} N^{25}} + \frac{\hat{\sigma}_a^{49} N^{49}}{\hat{\sigma}_a^{25} N^{25}}$$

$^{239}\text{Pu}_f$

$$\frac{dN_f^{49}}{dt} = \hat{\sigma}_f^{49} N^{49} \phi$$

$$\frac{dN_f^{49}}{dN^{25}} = - \frac{\hat{\sigma}_f^{49} N^{49}}{\hat{\sigma}_a^{25} N^{25}}$$

^{240}Pu :

$$\frac{dN^{40}}{dt} = \hat{\sigma}_c^{49} N^{49} \phi - \hat{\sigma}_a^{40} N^{40} \phi$$

$$\frac{dN^{40}}{dN^{25}} = - \frac{\hat{\sigma}_c^{49}}{\hat{\sigma}_a^{25}} \frac{N^{49}}{N^{25}} + \frac{\hat{\sigma}_a^{40}}{\hat{\sigma}_a^{25}} \frac{N^{40}}{N^{25}}$$

^{241}Pu :

$$\frac{dN^{41}}{dt} = \hat{\sigma}_a^{40} N^{40} \phi - \hat{\sigma}_a^{41} N^{41} \phi - \lambda^{41} N^{41}$$

$$\frac{dN^{41}}{dN^{25}} = - \frac{\hat{\sigma}_a^{40}}{\hat{\sigma}_a^{25}} \frac{N^{40}}{N^{25}} + \frac{\hat{\sigma}_a^{41}}{\hat{\sigma}_a^{25}} \left(1 + \frac{\lambda^{41}}{\hat{\sigma}_a^{41} \phi}\right) \frac{N^{41}}{N^{25}}$$

^{242}Pu :

$$\frac{dN^{42}}{dt} = \hat{\sigma}_c^{41} N^{41} \phi - \hat{\sigma}_a^{42} N^{42} \phi$$

$$\frac{dN^{42}}{dN^{25}} = - \frac{\hat{\sigma}_c^{41}}{\hat{\sigma}_a^{25}} \frac{N^{41}}{N^{25}} + \frac{\hat{\sigma}_a^{42}}{\hat{\sigma}_a^{25}} \frac{N^{42}}{N^{25}}$$

^{243}Am :

$$\frac{dN^{53}}{dt} = \hat{\sigma}_a^{42} N^{42} \phi - \hat{\sigma}_a^{53} N^{53} \phi$$

$$\frac{dN^{53}}{dN^{25}} = - \frac{\hat{\sigma}_a^{42}}{\hat{\sigma}_a^{25}} \frac{N^{42}}{N^{25}} + \frac{\hat{\sigma}_a^{53}}{\hat{\sigma}_a^{25}} \frac{N^{53}}{N^{25}}$$

^{244}Cm :

$$\frac{dN^{64}}{dt} = \hat{\sigma}_a^{53} N^{53} \phi - \hat{\sigma}_a^{64} N^{64} \phi - \lambda^{64} N^{64}$$

$$\frac{dN^{64}}{dN^{25}} = - \frac{\hat{\sigma}_a^{53}}{\hat{\sigma}_a^{25}} \frac{N^{53}}{N^{25}} + \frac{\hat{\sigma}_a^{64}}{\hat{\sigma}_a^{25}} \left(1 + \frac{\lambda^{64}}{\hat{\sigma}_a^{64} \phi}\right) \frac{N^{64}}{N^{25}}$$

where the symbols are defined in the same way as for plutonium fueled systems

except that N_f^{49} represents the ^{239}Pu fissions that have occurred. This quantity is obtained experimentally by subtracting the ^{235}U , ^{238}U , and ^{241}Pu fissions from the total fissions which is commonly obtained by measuring the ^{148}Nd or ^{37}Cs content of the burnup sample. This additional equation for the ^{239}Pu fissions leads to a much firmer least squares evaluation of $\hat{\alpha}^{49} = \hat{\sigma}_c^{49}/\hat{\sigma}_f^{49}$ than is possible without it. It should be noted that the production of ^{238}Pu from the alpha decay of ^{242}Cm has been neglected in the equation for ^{238}Pu . This is because ^{242}Cm decay is not uniquely describable in terms of the ^{235}U concentration, but depends more directly on the time variable which has been eliminated from the equations.. In practice, the generation of ^{238}Pu by ^{242}Cm decay is not negligible when compared with neutron capture in ^{237}Np . Thus, the

^{242}Cm decay contribution must be estimated and subtracted from the measured ^{238}Pu isotopic concentration in order to validate the above equation. The factors of one half that multiplies $\sigma_{n,2n}^{37}$ in the equation for dN^{46}/dt occurs because the $n,2n$ reaction for ^{237}Np generates ^{236}Np which, half of the time, undergoes β^- decay to ^{236}Pu while the remaining half decays to ^{236}U by electron capture, both decays possessing the same 22 hour half life.

If we assume that the cross section ratios are represented by

$$\begin{aligned} \hat{\sigma}_a^{28}/\hat{\sigma}_a^{25} &= A, \quad \hat{\sigma}_c^{25}/\hat{\sigma}_a^{25} = \beta, \quad \hat{\sigma}_a^{26}/\hat{\sigma}_a^{25} = b + bb/N^{26}, \quad \hat{\sigma}_{n,2n}^{28}/\hat{\sigma}_a^{25} = c, \\ \hat{\sigma}_a^{37}/\hat{\sigma}_a^{25} &= d, \quad \hat{\sigma}_a^{43}/\hat{\sigma}_a^{25} = e, \quad \hat{\sigma}_{n,2n}^{37}/\hat{\sigma}_a^{25} = f, \quad (\hat{\sigma}_a^{46}/\hat{\sigma}_a^{25})(1 + \lambda^{46}/\hat{\sigma}_a^{46} \phi) = g, \\ \hat{\sigma}_c^{28}/\hat{\sigma}_a^{25} &= B, \quad \hat{\sigma}_a^{49}/\hat{\sigma}_a^{25} = C + CC/N^{49}, \quad \hat{\sigma}_c^{49}/\hat{\sigma}_a^{25} = \epsilon, \quad \hat{\sigma}_a^{40}/\hat{\sigma}_a^{25} = D + DD/N^{40}, \\ (\hat{\sigma}_a^{41}/\hat{\sigma}_a^{25})(1 + \lambda^{41}/\hat{\sigma}_a^{41} \phi) &= E, \quad (\hat{\sigma}_c^{41}/\hat{\sigma}_a^{41})/(1 + \lambda^{41}/\hat{\sigma}_a^{41} \phi) = \gamma, \quad \hat{\sigma}_a^{42}/\hat{\sigma}_a^{25} = F, \\ \hat{\sigma}_a^{53}/\hat{\sigma}_a^{25} &= G, \quad \text{and} \quad (\hat{\sigma}_a^{64}/\hat{\sigma}_a^{25})(1 + \lambda^{64}/\hat{\sigma}_a^{64} \phi) = H \end{aligned}$$

then the differential equations in the second column on the preceding page can be integrated to yield

$$6. \quad N^{28} - K_8(N^{25})^A = 0$$

$$7. \quad N^{26} + \frac{\beta}{1-b} N^{25} + \frac{bb}{b} - K_6 (N^{25})^b = 0$$

$$8. \quad N^{37} - \frac{\beta b}{(1-b)(1-d)} N^{25} + \frac{bK_6}{(A-d)} (N^{25})^A + \frac{bK_6}{b-d} (N^{25})^b - K_7 (N^{25})^d = 0$$

$$\begin{aligned} 9. \quad N^{43} + \frac{\beta b d}{(1-b)(1-d)(1-e)} N^{25} - \frac{cdK_8}{(A-d)(A-e)} (N^{25})^A - \frac{bdK_6}{(b-d)(b-e)} (N^{25})^b + \frac{dK_7}{d-e} (N^{25})^d \\ - K_{48} (N^{25})^e = 0 \end{aligned}$$

$$\begin{aligned} 10. \quad N^{46} + \frac{Bbf}{2(1-b)(1-d)(1-g)} N^{25} - \frac{cfK_8}{2(A-d)(A-g)} (N^{25})^A - \frac{bfK_6}{2(b-d)(b-g)} (N^{25})^b \\ + \frac{fK_7}{2(d-g)} (N^{25})^d - K_{46} (N^{25})^g = 0 \end{aligned}$$

$$11. \quad N^{49} + \frac{BK_8}{A-C} (N^{25})^A - K_9 (N^{25})^C + \frac{CC}{C} = 0$$

$$12. \quad N_f^{49} - \frac{(1-\epsilon)BCK_8}{A-C} (N^{25})^A + (1-\epsilon) K_9 (N^{25})^C - K_{9f} = 0$$

$$13. \quad N^{40} - \frac{\epsilon BCK_8}{(A-C)(A-D)} (N^{25})^A + \frac{\epsilon CK_9}{C-D} (N^{25})^C - K_o (N^{25})^D + \frac{DD}{D} = 0$$

$$14. \quad N^{41} + \frac{\epsilon BCDK_8}{(A-C)(A-D)(A-E)} (N^{25})^A - \frac{\epsilon CDK_9}{(C-D)(C-E)} (N^{25})^C + \frac{DK}{D-E} (N^{25})^D - K_1 (N^{25})^E = 0$$

$$15. \quad N^{42} - \frac{\epsilon \gamma BCDEK_8}{(A-C)(A-D)(A-E)(A-F)} (N^{25})^A + \frac{\epsilon \gamma CDEK_9}{(C-D)(C-E)(C-F)} (N^{25})^C - \frac{\gamma DEK_o}{(D-E)(D-F)} (N^{25})^D \\ + \frac{\gamma EK_1}{E-F} (N^{25})^E - K_2 (N^{25})^F = 0$$

$$16. \quad N^{53} + \frac{\epsilon \gamma BCDEFK_8}{(A-C)(A-D)(A-E)(A-F)(A-G)} (N^{25})^A - \frac{\epsilon \gamma CDEFK_9}{(C-D)(C-E)(C-F)(C-G)} (N^{25})^C \\ + \frac{\gamma DEFK_o}{(D-E)(D-F)(D-G)} (N^{25})^D - \frac{\gamma EFK_1}{(E-F)(E-G)} (N^{25})^E + \frac{FK_2}{F-G} (N^{25})^F - K_3 (N^{25})^G = 0$$

$$17. \quad N^{64} - \frac{\epsilon \gamma BCDEFGK_8}{(A-C)(A-D)(A-E)(A-F)(A-G)(A-H)} (N^{25})^A + \frac{\epsilon \gamma CDEFGK_9}{(C-D)(C-E)(C-F)(C-G)(C-H)} (N^{25})^C \\ - \frac{\gamma DEFGK_o}{(D-E)(D-F)(D-G)(D-H)} (N^{25})^D + \frac{\gamma EFGK_1}{(E-F)(E-G)(E-H)} (N^{25})^E - \frac{FGK_2}{(F-G)(F-H)} (N^{25})^F \\ + \frac{GK_3}{G-H} (N^{25})^G - K_4 (N^{25})^H = 0$$

where, again, the K_i are constants of integration. The decay terms are evaluated from the equations

$$\frac{\lambda^{46}}{\sigma_a^{46} \phi} = \frac{\lambda^{46} \Delta t}{(\hat{\sigma}_a^{46} / \hat{\sigma}_a^{25}) \ln(N_o^{25} / N^{25})}, \quad \frac{\lambda^{41}}{\hat{\sigma}_a^{41} \phi} = \frac{\lambda^{41} \Delta t}{(\hat{\sigma}_a^{41} / \hat{\sigma}_a^{25}) \ln(N_o^{25} / N^{25})}, \text{ and}$$

$$\frac{\lambda^{64}}{\hat{\sigma}_a^{64} \phi} = \frac{\lambda^{64} \Delta t}{(\hat{\sigma}_a^{64} / \hat{\sigma}_a^{25}) \ln(N_o^{25} / N^{25})}.$$

Once the converged least squares fit has been attained and the isotopic concentrations and cross section ratios are known, the burnup in MWd/MTM (i.e., MegaWattDays per Metric Ton of heavy Metal) can be calculated from the total number of fissions occurring for each of the fissionable isotopes. The fissions by isotopes are

$$N_f^{25} = (1 - \hat{\sigma}_c^{25} / \hat{\sigma}_a^{25}) (N_o^{25} - N^{25})$$

$$N_f^{49} = N_f^{49}$$

$$N_f^{41} = (\hat{\sigma}_a^{41} / \hat{\sigma}_c^{41} - 1) (N^{42} + N^{53} + N^{64} - N_o^{42} - N_o^{53} - N_o^{64})$$

$$N_f^{28} = \delta_{25} N_f^{25} + \delta_{49} N_f^{49} + \sigma_{41} N_f^{41}$$

where 6_i is equal to the number of fissions that occur in ^{238}U because of fast neutrons from a fission in the i^{th} isotope. The 6_i are not determined from the least squares analysis and therefore must be supplied by the user. If we denote the number of MeV per fission for the i^{th} isotope by M^i , the burnup in MWD/MTM is

$$\text{BU} = C_{\text{BU}} (M^{25} N_f^{25} + M^{49} N_f^{49} + M^{41} N_f^{41} + M^{28} N_f^{28})$$

where C_{BU} is a conversion constant. If the N_f^i are in units of atoms/b-cm, then

$$C_{BU} = (1.602 \times 10^{-6} \frac{\text{erg}}{\text{MeV}}) (\frac{10^{-17} \text{ MWd}}{8.64 \text{ erg}}) (10^6 \frac{\text{gm U}}{\text{MTM}}) \frac{\frac{\text{b}}{\text{cm}^3}}{(\rho \frac{\text{gm U}}{\text{cm}^3})}$$

$$= \frac{1.854 \times 10^6}{\rho}$$

where ρ is the density of heavy metals (uranium plus plutonium) originally in the fuel.

The integrated burnup equations (1-17) are the theoretical equations which are fit to the isotopic burnup data (the N_f^i) by adjusting the least squares parameters (the A , b , B , ... ϵ , etc). These are divided into small groups of three to five equations and have been encoded as various versions of subroutine THEORY for use in DBUFIT-I. More explicitly the equation groupings are 1-3, and 3-5 for plutonium fuels and 6-10, 11-15, and 15-17 for uranium-plutonium fuels. Equations for the K_i which are evaluated with the first data point, have also been encoded.

ADAPTATION OF THE LIKELY LEAST SQUARES CODE
TO THE BURNUP PROBLEM

In the course of adapting the LIKELY least squares code to the burnup problem, an effort was also made to improve the efficiency and reliability of the code. Some of the changes are directly related to the burnup problem while others are of a more general nature. Some, but not all, of the changes can be found in DUBLIK⁽²⁾ which is the predecessor of DBUFIT-I.

First of all, modifications were made because of the simple form of the burnup equations. Notice that only two of the N^i occur in a given burnup equation (e.g. see Equations 1-5 and 6-17). One is associated with only that equation while the other (N^{49} for plutonium systems and N^{25} for uranium-plutonium systems) is common to all of the equations within its group. These burnup equations are much less complicated than the general equations LIKELY is able to handle (LIKELY can be used to solve problems for which each equation in a group is a function of all of the N^i of that group). Consequently, the burnup equations lead to simplifications within the code which reduce both computation time and core storage space.

Because of the efficient way in which the UNIVAC 1108 computer performs double precision computations, the LIKELY rounding routine FAMDR has been discarded, thereby eliminating the cumbersome FADR, FMPR, and FDPR functions from the encoded program. Many other minor alterations have been made. One of these was to increase the number of indices in the QPP and QYPP variables. Thus, these second derivatives with respect to the parameters are now described by two indices instead of a single "packed" index as in LIKELY. This change, when coupled with the new JUMP and N input variables, lends extra flexibility to the DBUFIT-I code. Consequently, the user is not forced to use all of the encoded burnup equations at once but can focus his attention

on one or two at a time without having to recode the THEORY subroutine. This feature proves useful for analyzing particularly difficult burnup problems because it permits the user to solve the problem in pieces that can later be used to obtain the complete solution. One other change is that the dimensions of the DBUFIT-I variables have been changed to allow the loading of the entire program into the UNIVAC 1108 memory at one time as opposed to the segmented LIKELY code.

Only one matrix inversion subroutine (INVERT) is used in DBUFIT-I. It proceeds with the matrix inversion by operating on the row and column keyed to the largest (in absolute magnitude) remaining diagonal element until the matrix has been reduced to the unit matrix. These diagonal "pivots" may be examined to test the matrix for positive-definiteness. The matrix is positive-definite if all of the diagonal pivots are positive.⁽⁵⁾ This information is important since one of the criteria for an acceptable solution to the least squares problem is that the misfit second gradient matrix be positive-definite. One other feature has been added to subroutine INVERT. This addition permits a selected parameter (or parameters) to be held fixed for a specified number of iterations (controlled by the LAG input variable) during the fitting process. If, for example, the 6th fitting parameter is to be held fixed for the first 10 iterations and allowed to vary from the 11th iteration onward, the program can be so instructed by setting LAG(6)=10.

The iterative scheme used in DBUFIT-I is considerably different than that used in LIKELY. The DBUFIT-I scheme will not proceed to the next iteration unless it knows how to get to a lower misfit (Q-value) than that of the current iteration. Several types of steps are used in an attempt to obtain a lower misfit. The first of these is the matrix step predicted from

the second order misfit expansion. The matrix step is the primary tool used to reduce the misfit in both the LIKELY and DBUPIT-I codes. It works extremely well when the matrix is positive-definite and is under the influence of the least squares best fit solution. However, these conditions are seldom realized during the initial iterations because fitting parameter guesstimates are rarely that accurate. In this situation the gradient and/or reversed matrix steps are frequently the most productive.⁽⁶⁾ In many cases, fractional steps of one type or another are also helpful. The parameter changes predicted by each type of step are used to generate a new Q-value. If this new Q-value is lower than that of the current iteration, the parameters predicted by this type of step are used for the next iteration. However, if the new Q-value is larger than or equal to the current Q-value, the next type of step is tried. The Iterative process continues until either the change in the Q-value is less than one part in 10^5 and the second derivative of the misfit is positive-definite (this is the program definition of convergence), or none of the step types yield a lower Q-value, in which case the iterative loop is terminated and the step type is labeled FINI. The gradient and reversed matrix steps have been found to be both reliable and efficient in directing the iterative least squares path toward convergence when the matrix step fails to do so. On the other hand, once the iterative process is thereby brought under the influence (i.e., in the immediate vicinity) of the converged fit, the matrix step quickly homes in on the converged fit. The program logic for the iterative loop is shown in Figure 1.

The probability calculations (subroutines WORIH and ERF) of LIKELY have been eliminated from DBUFIT-1 in order to reduce computation time. As a result, a decision as to the acceptability of a data point has been changed.

$DQUEST$ = CHANGE IN Q PREDICTED BY THE MATRIX STEP
 $INDEF$ $\begin{cases} = 0 & \text{IF MATRIX IS POSITIVE-DEFINITE} \\ > 0 & \text{IF MATRIX IS INDEFINITE} \end{cases}$
 ΔQ = ACTUAL CHANGE IN Q

Figure 1. Normal Iterative Mode of Traversing DBUFIT-I.

A data point is now labeled as "BAD" if its mean square misfit is more than the average mean square misfit of the other points multiplied by the program variable BAD. The user can override the preset value of $BAD=3$ via input data. If BAD is negative in sign, data points labeled as "BAD" will be deleted and the remaining data will be rerun through the least squares fitting routine.

THE APPLICATION OF THE DBUFIT-I CODE
TO A BURNUP PROBLEM

This section is concerned with the application of the DBUFIT-I code to burnup data. The specifics involved in the use of the code are illustrated by setting up and discussing the results of a sample burnup case. Additional general comments that may be of aid to the user are also offered.

INPUT

The burnup equations that are most frequently used are the plutonium equations for uranium-plutonium systems (i.e., Equations 11-15). The sample case consists of burnup data obtained from exposed $\text{UO}_2\text{-PuO}_2$ fuel that is applicable to these equations. There are nine data points, of which the first one is the zero burnup point (i.e., the isotopic concentration data for this point are those of the unirradiated fuel). A set of general input instructions for the code are listed on "comment" cards in the main program and are reproduced in Table I. Notice that many of the program variables are preset to a given value by the program. The user, however, can override these preset values with those of his own via input cards.

The burnup equations are entered **into the** program **via** subroutine THEORY. The formulation of these equations are explained on "comment" cards listed at the beginning of this subroutine. The relationships of (a) the parameters with the cross section ratios and isotopic concentrations of the first data point, and (b) the $Z(M,I)$ with the isotopes and burnup are also shown on these cards. These comment cards are reproduced in Table II. The burnout equations come first and appear as "Q" equations. The constants of integration involved in these equations are shown next. These "R" expressions are the K_i of Equations 11 through 15. Next appear the relationships between the Z's and

TABLE IGENERAL INSTRUCTIONS FOR
PROGRAM DBUFIT-I

C NAMELIST INPUT LIST

```

C$INPUT
C  IL=      ITERATION LIMIT (MINIMUM 0, NO MAXIMUM, TRY 7)          PRESET 0
C  IX=      NUMBER OF PRECISE X-COORDINATES (MINIMUM 0, MAXIMUM 7-JY) PRESET 0
C  JUMP=     NUMBER OF Q EQUATIONS TO BE JUMPED OVER                PRESET 0
C  JY=      NUMBER OF IMPRECISE Y-COORDINATES (MINIMUM 1, MAXIMUM 6) PRESET 1
C  KP=      NUMBER OF PARAMETER P-COORDINATES (MINIMUM 1, MAXIMUM 15) PRESET 1
C  LQ=      NUMBER OF MISFIT Q-COORDINATES (MINIMUM 1, MAXIMUM 5)   PRESET 1
C  MM=      NUMBER OF MEASUREMENT VECTORS Z(M) (MINIMUM 1, MAXIMUM 150) PRESET 1
C  N=       PARAMETERS N+1 THROUGH N+KP ARE VARIED WITH REMAINDER FIXED PRESET 0
C  NC=      NUMBER OF CONSTANTS OR CONTROLS C (MINIMUM 01 MAXIMUM 25) PRESET 0
C  C(1)=    THEORY CONSTANTS OR MULTIPLE-THEORY CONTROLS

C          PROGRAM CONTROLS (0=CONTROL OFF, 1=CONTROL ON) WHEN CONTROL IS ON
C  LIKCON(1) SUPPRESSES PRINTOUT OF MEASUREMENT DATA
C  LIKCON(2) CONTROLS THE METHOD OF HANDLING THE INITIAL CONCENTRATIONS
C           0 INCLUDE INITIAL CONCENTRATIONS AS VARIABLE PARAMETERS
C           1 INITIAL CONCENTRATION PARAMETER GUESSTIMATES CALCULATED FROM
C             FIRST DATA POINT
C           2 INITIAL CONCENTRATION PARAMETERS HELD FIXED AT VALUE OF
C             FIRST DATA POINT
C  LIKCON(3) CONTROLS ITERATIVE LOGIC IN SUBROUTINE MINMAX
C           0 (SERIES APPROACH) USE FIRST STEP IN SERIES (MATRIX, MATRIX/2,
C             -MATRIX/2, GRADIENT) THAT YIELDS A DROP IN QQ
C           1 (PARALLEL APPROACH) TYPE OF STEP THAT YIELDS LOWEST QQ IS USED
C  LIKCON(4) BYPASS FULL MATRIX STEP IF MATRIX IS INDEFINATE
C  LIKCON(5) CALCULATE ONE STANDARD DEVIATION ERROR OF CROSS SECTION RATIOS
C  LIKCON(6) YYPASSES ERROR ANALYSES AND PLOTS
C  LIKCON(7) PUNCHES PARAMETERS FOR RESTART
C  LIKCON(8) CONTROLS PRINTOUT OF PARAMETER UNCERTAINTY INFORMATION AND
C             MATRIX INVERSION CHECK
C           1 PRINT PARAMETER VARIANCE-COVARIANCE MATRIX .DPDP=
C           2 PRINT 1 PLUS PARAMETER UNCERTAINTY CORRELATION MATRIX
C           3 PRINT 2 PLUS MATRIX INVERSION CHECK
C  BAD=     A POINT IS LABELED BAD IF ITS MISFIT IS MORE THAN BAD(SAY 3.)
C           TIMES THE AVERAGE MISFIT OF THE OTHER POINTS          PRESET 3
C           MINUS BAD MEANS (DISCARD BAD DATA, SET BAD PLUS, RUN REFIT)
C  P(1)=    PARAMETER ESTIMATES P(K), K=1,20
C           WARNING...ONLY 15 PARAMETERS CAN BE VARIED (I.E. KP.LE.15)
C  LAG(1)=  ITERATIONS TO LAG BEFORE PARAMETER VARIATION LAG(K), K=1,20 PRESET 0
C  Z(1,1)=  MEASUREMENTS (Z(M,JI), M=1,MM), JI=1,JY+IX          PACKED VECTORS

```

TABLE I (Cont'd)

```

C      IMPRECISE(Y(M,J),M=1,MM),J=1,JY PRECISE(X(M,I),M=1,MM),I=1,IX
C U(1,1)= MEAN SQUARE CORRELATED MEASUREMENT UNCLKTAINTY U(M,J1J2)
C      ((U(M,J1,J2),M=1,MM),J2=J1,JY),J1=1,JY PACKED 11NSORS
C UGEN= NOT -0. GENERATE UNCERTAINTY U(M,J,J)=Y(M,J)**UGEN PRESET-0
C UEXP= NOT -0. EXPONENTIATE U(M,J1,J2)=U(M,J1,J2)**UEXP PRESET-0
C YEXP= NOT -0. DO U(M,J1,J2)=U(M,J1,J2)*(Y(M,J1)*Y(M,J2))**YEXP PRESET-0

C MAP= THEORY-MEASUREMENT HYPER-SPACE PLOTS (NONE ~,MAX MUM3) PRESET 0
C MAP$(PLOTTER) SUBROUTINE HAS FOLLOWING REQUIREMENTS
C 1 THERE IS ONLY ONE INDEPENDENT VARIABLE--5AY ZA
C 2 THEORY Q EQUATIONS ARE OF FORM Z(I)-FN(ZA)=0, I.NE.A
C 3 THERE SHOULD BE JY+IX ZDZSDS INPUT CARDS
C 4 A VARIABLE IS EXCLUDED FROM A PLOT BY SETTING POSITION 5 OF IT5
C ZDZSDS CARD TO A NEGATIVE NUMBER
C A Y VARIABLE IS AUTOMATICALLY EXCLUDED FROM THE PLOT IF IT WAS
C NOT INCLUDED IN THE FIT
C 5 ONLY LINEAR SCALES ARE ALLOWED
C ZDZSDS(1,1,1)=((Z-SCALE(Z1,DZ,Z2)=(S1,DS,S2)INCHES,J1=1,JY+IX),M=1,MAP
C FIRST INDEX=PLOT SCALE, SECOND=COORDINATE INDEX,THIRD=PLOT NUMYER
C DZ.NE.0. INDEPENDENT-VARIABLE
C DZ=0. DEPENDENT-VARIABLE
C DS.GT.0. VARIABLE IS PLOTTED ON THE X-AXIS
C DS=0. VARIABLE IS PLOTTED ON THE Y-AXIS
C DS.LT.0. VARIABLE IS NOT PLOTTED
C OFF-SCALE POINTS ARE PROJECTED TO THE NEAREST BOUNDARY

C PLOT CONTROLS (0=CONTROL OFF, 1=CONTROL ON) WHEN CONTROL IS ON
C MAPCON(1) PRINTS OUT NUMERIC TABLES OF THE PLOT
C MAPCON(2) PLOTS SYMBOL AT EACH DATA POINT
C MAPCON(3) PLOTS ONE STANDARD DEVIATION UNCERTAINTY FOR EACH DATA POINT
C MAPCON(4) PLOTS FITTED CURVE
C MAPCON(5) PLOTS ONE STANDARD DEVIATION UNCERTAINTY OF FITTED CURVE
C MARK= PLOT SYMBOL INDICATOR MINUS MARK SUPERIMPOSES PLOTS
C $ END OF CASE

C TO TERMINATE RUN AT END OF CURRENT ITERATION,DEPRESS SENSE SWITCH 1
C AT END OF RUN, PARAMETERS P(K) ARE BEST VALUES, UGEN=UEXP=YEXP=-0.,

```

TABLE II

A LISTING OF THE ENCODED PLUTONIUM **BURNUP** EQUATIONS
FOR URANIUM-PLUTONIUM SYSTEMS

```

C_ GENERALIZED THEORY EQUATIONS FOR URANIUM-PLUTONIUM SYSTEMS
C   Q1=Z2+P3*Z1**P2-R1*Z1**P4+P5
C
C   Q3=P7*Z4+P7*P10-P3*Z1**P2/((P2-P9)+R1*Z1**P4/(P4-P9))-R3*Z1**P9
C_ Q4=P7*Z5/P9+P3*Z1**P2/((P2-P9)(P2-P12))-R1*Z1**P4/((P4-P9)(P4-P12))+
C   R3*Z1**P9/(P9-P12)-R4*Z1**P12
C_ Q5=P7*P14*Z6/(P9*P12)-P3*Z1**P2/((P2-P9)(P2-P12)(P2-P16))+
C   R1*Z1**P4/((P4-P9)(P4-P12)(P4-P16))-R3*Z1**P9/((P9-P12)(P9-P16))+
C_ R4*Z1**P12/(P12-P16)-R5*Z1**P16
C_ CONSTANTS OF INTEGRATION(EVALUATED AT Z1=Z(1,1)=U235 FOR FIRST DATA POINT)
C_ R1=(P6+P3*Z1**P2+P5)/Z1**P4
C   R2=P7*P8/(P4*P7-1)-P3*Z1**P2/P2+R1*Z1**P4/P4
C_ R3=(P7*P11+P7*P10-P3*Z1**P2/((P2-P9)+R1*Z1**P4/(P4-P9)))/Z1**P9
C   R4=(P7*P13/P9+P3*Z1**P2/((P2-P9)(P2-P12))-R1*Z1**P4/((P4-P9)(P4-P12))+
C_ R3*Z1**P9/(P9-P12))/Z1**P12
C   R5=(P7*P14*P15/(P9*P12-P3*Z1**P2/((P2-P9)(P2-P12)(P2-P16))+
C_ R1*Z1**P4/((P4-P9)(P4-P12)(P4-P16))-R3*Z1**P9/((P9-P12)(P9-P16))+
C   R4*Z1**P12/(P12-P16))/Z1**P16

C_ Z(M,1)  Z(M,2)  Z(M,3)  Z(M,4)  Z(M,5)  Z(M,6)  Z(M,7)
C   U235    PU239    PU239FIS  PU240    PU241    PU242    BURNUP

C_ P1      P2      P3      P4      P5      P6
C   BU238  RHO    ALF8*RHO*BU238/((RHO-A)*BU235**RHO)  A  AA/A  BPU249
C_ P7      P8      P9      P10     P11     P12     P13     P14     P15  P16
C   1/(ALF9*A)  BPU249F  B  BB/B  BPU240  C*C(6)  BPU241  C(6)/ALF1  BPU242  3

C_ WHERE XC28/XA28=ALF8  XA28/XA25=RHO  XA49/XA25=A+AA/N49
C_ XC49/XA49=ALF9  XA40/XA25=B+BB/N40  XA41/XA25=C
C_ XC41/XA41=ALF1  XA42/XA25=D

C_ C(1)=BURNUP IN MWD/MTM OF THE FIRST DATA POINT
C_ IF C(1).LT.0 OMIT BURNUP CALCULATIONS
C_ CONVERSION CONSTANT DEPENDING ON THE FOAM OF THE ZS
C_ C(2)=185.416 IF Z=ATOMS/GM OF HEAVY METAL X 10**-20
C_ C(2)=185.416/DEN IF Z=ATOMS/B-CM X 10**4 DEN=DENSITY OF HEAVY METAL
C_ C(3)=U235 MEV/FIS+DEL235*U238 MEV/FIS
C_ C(4)=PU239 MEV/FIS + DEL239*U238 MEV/FIS
C_ C(5)=PU241 MEV/FIS+DEL241*U238 MEV/FIS
C_ C(6)=1+LAMBDA41/(SIGA41*PHI)
C_ C(7)= ONE STANDARD DEVIATION ERROR OF LAMBDA41/(SIGA41*PHI)
C_ C(8)= ALPHA235
C_ C(9)= ONE STANDARD DEVIATION ERROR OF ALPHA235

C_ JUMP=NUMBER OF Q EQUATIONS TO BE JUYPED OVER
C_ PARAMETERS...FIRST N FIXED,NEXT KP VARIED,AND REMAINDER FIXED

```

the isotopes and then between the parameters and the cross section ratios and initial concentrations. Finally, various constants used in the program are explained. For example, the density of the uranium plus plutonium in the unexposed fuel is 8.315 gm/cm^3 , thus $C(2) = 185.416/8.315 = 22.999 \approx 22.3$ is entered as part of the input data. In calculating $C(3)$, $DEL235 =$ fissions induced in ^{238}U due to fast neutrons from a ^{235}U fission. Similar definitions hold for $DEL239$ and $DEL241$. The quantity entered in $C(8)$ is $ALPHA235 = \hat{\sigma}_c^{25}/\hat{\sigma}_f^{25}$.

The FORTRAN-V equations for the burnup equations and their derivatives have not been included in Table II. There are almost 600 of them of which almost ninety percent are related to the derivatives. If the user wishes to see these equations he can do so by listing subroutine THEORY. Similar subroutines have been developed for the burnup Equations 1-3, 6-10, and 15-17. "Comment" cards at the beginning of these subroutines are again used to orient and inform the user how to set up the input data.

The deck of punched cards used to run the sample problem is shown in Table III. The first and last lines are not part of the deck, They are included so that the column numbers of the input deck can be ascertained from the table. The cards labeled SYS are required by the executive program of the local UNIVAC-1108 computer. Cards are included which modify the "dummy" ARTIST subroutine so that appropriate scales and titles are recorded on the axes of the graphical output. The program execution card is tagged with a "U" (located after XQT) which calls into use those program subroutines that apply to uranium-plutonium burnup systems. A "P" replaces the "u" for systems containing only plutonium fuel.

The input data is sandwiched between the \$INPUT and \$ cards according to a NAMELIST format. The values assigned to the input variables are in accord with the instructions and relationships of Tables I and II. The parameter

TABLE III

A LISTING OF THE INPUT CARDS
FOR THE SAMPLE BURNUP CASE

```

*****1*****2*****3*****4*****5*****6*****7*****8
' RUN 5,CUS114, ,200,2000 RP MATSEN SYS
'X ASG A=U0792 - SYS
' ASG,W H=(,NH,AT) SYS
' XQT CUR -----SYS
IN 4 SYS
TRI 4 -----SYS
'IT FR5,* ARTIST,ARTIST SYS
-1 -----SYS
    DIMENSION AXES(5,6),TITLE(7,6),TITL(7)
    DATA AXES/ 0.,0.,10.,0.,1., ,5., 5., 7., 2.,4.,.2,
1      0., 0.,12.,.2.,.05, 10.,0.,12.,0.,.02,
2      10.,5., 0.,.12.,0.,.25, ,10.,0.,12.,0.,.25 /
    DATA TITLE/
147H BURNUP (UNITS' GWD/MTM) - ,---
242H PU-239 (UNITS' .0001 ATOMS/B-CM) ,
342H PU-240 (UNITS' .0001 ATOMS/B-CM) ---
442H PU-241 (UNITS' .0001 ATOMS/B-CM) ,
542H PU-242 (UNITS' .000001 ATOMS/B-CM) ---
642HPU-239 FISSIONS (UNITS' .0001 ATOMS/B-CM) /
    DATA TITL/42H U-235 (UNITS' .0001 ATOMS/B-CM) --- /
    J1=5
    IF(ND.EQ.0) GO TO 100
    DO 50 I=1,7
50 TITLE(I,1)=TITL(I)
    AXES(3,1)=9.
    AXES(4,1)=1.5
    AXES(5,1)=-.05
    AXES(1,4)=9.
    AXES(1,5)=9.5
    AXES(1,6)=10.5
C DO (TIC5 SCALES TAGS) AXIS(X,Y,TAG,NH,SPAN,ANGLE,DATA1,DATA/INCH)
100 DO 200 J=1,J1
    LABEL=-42
    IF(J.EQ.2.OR.J.EQ.3) LABEL=42
    ANGLE=90.
    IF(J.EQ.1) ANGLE=0.
    200 CALL AXIS(AXES(1,J),AXES(2,J),TITLE(1,J),LABEL,AXES(3,J),ANGLE,AXE
    1S(4,J),AXES(5,J))
    ND=1
! MSG 300 PAPER FLUID INK PEN SYS
! MSG LABEL TAPE H. PLOT TAPE H ON CALCOMP SYS

```

TABLE III (Cont'd)

```

! MSG R P MATSEN CUS114 ROB BLDG 3000 AREA-
!N XQT,U DBUFIT
$INPUT
IL=25,
MM=9, JY=6, IX=1,
LQ=5, JUMP=0, N=2, KP=13,
NC=9, C(1)=0.,22.3,212.87,222.32,225.14,1.11,.03,.2197,.0009,
P(1)=
204.678,.01604132678619039,-1.5,2.,0.,0.,1.5,0.,1.4,0.,0.,2.5,0.,
4.2585,0.,.4102,
LIKCON(2)=1,2*0,1,0,1,2,
LAG(14)=99,
Z(1,1)=
.14851+01, .14056+01, .13824+01, .13557+01, .13058+01, .12690+01,U-235
.12376+01, .11910+01, .11196+01,
Z(1,2)=
.37910+01, .34604+01, .34692+01, .33290+01, .32066+01, .31518+01,PU239
.30038+01, .28481+01, .26766+01,
Z(1,3)=
.00000 , .24449-00, .34452-00, .47442-00, .64316-00, .74723-00,PU239F
.85647-00, .10613+01, .12801+01,
Z(1,4)=
.34460-00, .43324-00, .47529-00, .50900-00, .57654-00, .61461-00,PU240
.64613-00, .69920-00, .77700-00,
Z(1,5)=
.47701-01, .70962-01, .84476-01, .97209-01, .11730+00, .13040-00,PU241
.13863-00, .16215-00, .19628-00,
Z(1,6)=
.33323-02, .50176-02, .60018-02, .72904-02, .98667-02, .11567-01,PU242
.13619-01, .17891-01, .25047-01,
Z(1,7)=
.00000 , .15443+04, .21381+04, .29037+04, .39614+04, .46471+04,BU
.53380+04, .65856+04, .80483+04,
U(1,1)=
.22000-05, .81200-05, .30979-05, .96432-05, .96294-05, .96191-05,ERR55
.96179-05, .96040-05, .80548-05,
U(1,7)=
.14396-02, .36404-02, .35309-02, .33537-02, .28408-02, .27430-02,ERR99
.24852-02, .22387-02, .19737-02,
U(1,9)=
.12820-03, .45578-03, .48373-03, .51278-03, .51077-03, .53489-03,ERR90
.53456-03, .54961-03, .57298-03,
U(1,10)=
.18050-04, .74654-04, .85977-04, .97932-04, .10391-03, .11348-03,ERR91
.11469-03, .12746-03, .14474-03,
U(1,11)=
.12600-05, .52820-05, .61123-05, .73477-05, .87484-05, .10072-04,ERR92
.11279-04, .14076-04, .18492-04,

```

TABLE III (Cont'd)

```

U(1,12)=
.10000-19, .71232-04, .84050-04, .17275-03, .21290-03, .29737-03,ERRP9F
.35598-03, .51102-03, .74609-03,
U(1,16)=
.14300-04, .58980-04, .68197-04, .81175-04, .10017-03, .11424-03,ERR00
.12590-03, .14661-03, .18245-03,
U(1,17)=
.16080-05, .93467-05, .11779-04, .14974-04, .18684-04, .22129-04,ERR01
.24670-04, .31291-04, .42018-04,
U(1,18)=
.11230-06, .66131-06, .83739-06, .11235-05, .15730-05, .19641-05,ERR02
.24262-05, .34557-05, .53682-05,
U(1,19)=
.29600-06, .16653-05, .22880-05, .31037-05, .42840-05, .51205-05,ERR11
.57861-05, .79243-05, .11605-04,
U(1,20)=
.15800-07, .10832-06, .14884-06, .21456-06, .32001-06, .41671-06,ERR12
.52054-06, .80139-06, .13561-05,
U(1,21)=
.67150-08, .12454-07, .15395-07, .20531-07, .36822-07, .44774-07,ERR22
.69464-07, .10642-06, .20835-06,
U(1,22)=
.10000+01, .59623+04, .11429+05, .21079+05, .39232+05, .53990+05,ERRBU
.71234+05, .10842+06, .16194+06,
MAP=2, MAPCON(1)=5*1,
ZDZSDS(1,1,1)=1.5, -.025, 1.05, 0., -.5, 8.,
ZDZSDS(1,2,1)= 4., 0., 1.4, 13., 0., 0.,
ZDZSDS(1,3,1)= 0., 0., 3.25, 0., 0., 13.,
ZDZSDS(1,4,1)= .2, 0., .85, 0., 0., 13.,
ZDZSDS(1,5,1)= 0., 0., .26, 0., 0., 13.,
ZDZSDS(1,6,1)= 0., 0., .0325, 0., 0., 13.,
ZDZSDS(1,7,1)= 0., 0., 10000., 0., 1., 10.,
ZDZSDS(1,1,2)=1.5, -.025, 1.05, 0., .5, 8.,
ZDZSDS(1,2,2)= 4., 0., 1.4, 13., 0., 0.,
ZDZSDS(1,3,2)= 0., 0., 3.25, 0., 0., 13.,
ZDZSDS(1,4,2)= .2, 0., .85, 0., 0., 13.,
ZDZSDS(1,5,2)= 0., 0., .26, 0., 0., 13.,
ZDZSDS(1,6,2)= 0., 0., .0325, 0., 0., 13.,
ZDZSDS(1,7,2)= 0., 0., 10000., 0., -1., 10.,
$
! FIN
*****1*****2*****3*****4*****5*****6*****7*****8

```


guesstimates were arrived as follows. The parameters P(1) and P(2) have previously been obtained from a least squares fit of the ^{238}U vs. ^{235}U data. The parameter P(1) is not used in the current fit. The parameter P(2) is used in the fit but it is not permitted to vary. Holding these first two parameters fixed is accomplished by setting $N = 2$. Guesstimates for the parameters P(6), P(8), P(11), P(13), and P(15) are internally set by the program as a result of setting $\text{LIKCON}(2) = 1$. They are set at the values of the first data point, i.e., $P(6) = ^{239}\text{Pu}$, $P(8) = ^{239}\text{Pu}_f$, $P(11) = ^{240}\text{Pu}$, $P(13) = ^{241}\text{Pu}$, and $P(15) = ^{242}\text{Pu}$. Since the program (when $\text{LIKCON}(2) = 1$) generates guesstimates for these parameters, we can insert any value (in this case zero) for them. If $\text{LIKCON}(2) = 0$, good guesstimates must be supplied for these parameters. If $\text{LIKCON}(2) = 2$, the guesstimates are supplied as in the case of $\text{LIKCON}(2) = 1$ with the added provision that these parameters are not allowed to vary, thereby forcing the fit to pass through the first data point. The guesstimates for the parameters which are related to the cross section ratios are shown in Table IV. The guesstimates for the cross section ratios are shown in the left column and the corresponding parameter guesstimates are to the right.

Notice that parameters P(14) and P(16) have their guesstimates set at their best known values. This is because they are held fixed during the iterative process. Thus, their initial value will also be their final value. The input variable $\text{LAG}(14) = 99$ holds P(14) fixed and P(16) is not varied because only the KP parameters after the first N parameters are varied (i.e., $N + \text{KP} = 15$ and therefore P(16) is not varied). An explanation of the reason for holding P(14) and P(16) fixed is given later on. Because of the way that the cross section ratio parameters occur in the buraup equations, no two of these parameter guesstimates should have the same value.

TABLE IV

PARAMETER GUESSTIMATES FOR THE SAMPLE CASE

<u>Cross Section Ratio Guesstimates</u>	<u>Parameter Guesstimates</u>
$\hat{\sigma}_c^{28}/\hat{\sigma}_a^{25} = 0.015$	$P(3) = \frac{(0.015)(204.678)}{(0.016-2.)(1.4851)^{0.016}}$ $= -1.5377 \approx -1.5$
$\hat{\sigma}_a^{49}/\hat{\sigma}_a^{25} = 2$	$P(4) = 2.0$ and $P(5) = 0.0$
$\hat{\sigma}_d^{49} = \hat{\sigma}_d^{49}/\hat{\sigma}_f^{49} = 0.5$ or $\hat{\sigma}_c^{49}/\hat{\sigma}_a^{49} = 0.333$	$P(7) = \frac{1.0}{(0.333)(2.0)} = 1.5$
$\hat{\sigma}_a^{40}/\hat{\sigma}_a^{25} = 1.4$	$P(9) = 1.4$ and $P(10) = 0.0$
$\hat{\sigma}_a^{41}/\hat{\sigma}_a^{25} = 2.25$	$P(12) = 2.25 (1.11) = 2.5$
$\hat{\sigma}_c^{41} = \hat{\sigma}_c^{41}/\hat{\sigma}_f^{41} = 0.35254$ or $\hat{\sigma}_c^{41}/\hat{\sigma}_a^{41}$ $= 0.26065$	$P(14) = \frac{1.11}{0.2607} = 4.2585$
$\hat{\sigma}_a^{42}/\hat{\sigma}_a^{25} = 0.4102$	$P(16) = 0.4102$

Some sets of burnup data do not readily lead to a converged fit when set up as shown in Table III. However, such data will often yield to a sequence of least squares runs by fitting only a few equations at a time. In this way, good parameter estimates are obtained for the final run which consists of a simultaneous fit of all the equations to the data. Table V suggests such a series of runs.

TABLE V

SEQUENTIAL RUNS FOR DIFFICULT BURNUP PROBLEMS

Run	<u>Input Changes</u>	<u>Fitted Burnup Equations</u>	<u>Parameters Determined by fit</u>
1	LQ=3, JUMP=0, N=2, KP=9, LAG(9)=99, 99,	^{239}Pu , $^{239}\text{Pu}_f$, ^{240}Pu	P(3), P(4), P(5), P(6)
2	LQ=3, JUMP=1, N=6, KP=7, LAG(9)=3*0, 99,	$^{239}\text{Pu}_f$, ^{240}Pu , ^{241}Pu	P(7), P(8)
3	LQ=3, JUMP=2, N=8, KP=7, LAG(12)=2*0, 99,	^{240}Pu , ^{241}Pu , ^{242}Pu	P(9), P(10), P(11), P(12), P(13), P(15)
4	LQ=5, JUMP=0, N=2, KP=13, LAG(14)=99,	All	All except P(14)

For the sequence of runs shown in Table V, the MAP and ZDZSDS variables used to obtain plots of the fitted data are excluded from the input of all runs except the final one.

The isotopic concentration data along with their variance-covariance matrices are entered in the Z and U variables. The isotopic concentrations entered into the Z(M,I) are in atoms/b-cm multiplied by 10^4 (i.e., the numbers are in units of 10^{-4} atoms/b-cm). The variance-covariance values entered as U(M,I) variables have been multiplied by a corresponding value of 10^8 . The U variables involve "packed" indices so an example of how they are put together is in order. The variance-covariance matrices (the variance of number is simply the square of its one standard deviation uncertainty) for the first two data points are

	U235	Pu239	Pu239 _f	Pu240	Pu241	Pu242
U235	2.2-6	0	0	0	0	0
Pu239	0	1.4396-3	0	1.282-4	1.805-5	1.260-6
Pu239 _f	0	0	1.0-20	0	0	0
Pu240	0	1.2820-4	0	1.430-5	1.608-6	1.123-7
Pu241	0	1.8050-5	0	1.608-6	2.960-7	1.580-8
Pu242	0	1.2600-6	0	1.123-7	1.580-8	6.715-9

and

U235	Pu239	Pu239 _f	Pu240	Pu241	Pu242
8.12-6	0	0	0	0	0
0	3.6404-3	0	4.5578-4	7.4654-4	5.2820-6
0	0	7.12 32-5	0	0	0
0	4.5578-4	0	5.8980-5	9.3467-6	6.6131-7
0	7.4654-5	0	9.3467-6	1.6653-6	1.0832-7
0	5.2820-6	0	6.6131-7	1.0832-7	1.2454-8

These matrices are symmetric. Therefore, all of the information can be entered into the program by excluding those elements below the diagonal. Thus, the elements of the variance-covariance matrix for the Mth data point, symbolically shown below, corresponds to the U variables as indicated.

1,1	1,2	1,3	1,4	1,5	1,6	U(M,1)	U(M,2)	U(M,3)	U(M,4)	U(M,5)	U(M,6)
	2,2	2,3	2,4	2,5	2,6		U(M,7)	U(M,8)	U(M,9)	U(M,10)	U(M,11)
		3,3	3,4	3,5	3,6			U(M,12)	U(M,13)	U(M,14)	U(M,15)
			4,4	4,5	4,6				U(M,16)	U(M,17)	U(M,18)
				5,5	5,6					U(M,19)	U(M,20)
					6,6						U(M,21)

Thus

$$U(1,1) = 2.2-6, 8.12-6, \dots$$

$$U(1,7) = 1.4396-3, 3.6403-3, \dots$$

$$U(1,13) = 1.-20, 7.1232-5, \dots$$

All of the values for U(M,2), U(M,3), U(M,4), U(M,5), U(M,6), U(M,8), U(M,13), U(M,14), and U(M,15) are zero. Therefore, they need not be specifically entered as part of the input data. The values entered for U(M,22) are variances of the burnup variable, Z(M,7). Their sole use is to formulate error flags on the burnup values displayed in the first plot (see Figure 2). The input data required for the plots is described later.

OUTPUT

The DBUFIT-I output for the sample case consists of (1) printed output, (2) two plots, and (3) seven cards with the final parameters punched on them. The printed output is shown in Table VI. The numerical output begins after a listing of the compiled ARTIST subroutine. The first part of the numerical output is a listing of the input data. This is written out in order to provide a record of the input data. If it is desired, the printout for the measurement vectors and mean square correlated-measurement-uncertainty tensors (variance-covariance matrices) can be omitted by setting $\text{LIKCON}(1) = 1$,

Information pertaining to the iterative process makes up the next part of the output. For the sample case, a converged fit was obtained after thirteen iterations which is somewhere near average when fairly good parameter guesstimates are used. The only step types required for this case were the matrix and half-matrix steps. In the more difficult problems the gradient and reversed-half-matrix steps are also used, as depicted in Figure 1. If none of these step types yield a reduction in the misfit then the step type is labeled FINI and the iterative process is terminated. If this occurs, the user should check to see that his input data is correct. If it is, the case should be rerun with new (and hopefully better) parameter guesstimates. A least squares minimum is attained when the misfit gradient vanishes and the misfit second gradient is **positive-definite** (signaled by positive values for all of the matrix inversion blade pivots). If one or more of the blade pivots is negative, that particular iteration is on or under the influence of a real or imaginary saddle type of solution. At any rate, such a solution is not acceptable for least squares problems.

LOG NUMBER = 8B0210

'0 RUN 5,CUS114, ,200,2000 RP MATSEN

'X ASG A=U0792 8B0210

TAPE ASSIGNMENTS A= 4/03 U0792

' ASG,W H=(,NH,AT)

TAPE ASSIGNMENTS H= 4/00 U1532

' XQT CUR

1. IN A

END FILE --- UNIT A

2. IRI A

END CUR

SYS

SYS

SYS

SYS

SYS

SYS

PRINTED OUTPUT FOR THE SAMPLE CASE

TABLE VI

30

!IT FR5,* ARTIST,ARTIST
 UNIVAC 1108 FORTRAN V LEVEL 2206 0009 F600A - CSC005
 THIS COMPILATION WAS DONE ON 31 MAR 70 AT 11:56:53

SYS

--- SUBROUTINE ARTIST ENTRY POINT 000143

STORAGE USED (BLOCK, NAME, LENGTH)

0001	*CODE	000162
0000	*DATA	000156
0002	*BLANK	000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003	AXIS
0004	NEHR35

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000024	100L	0001	000006	116G	0001	000032	131G	0000 R	000125	ANGLE	0000 R	000000	AXES	
0000	1	000122	0000	000117	IS	0000	000123	J	0000	1	000120	J1	0000	000124	LABEL
0000	000121	ND	0000 R	000110	TITL	0000 R	000036	TITLE							

TABLE VI (Cont'd.)

1.	00101	SUBROUTINE ARTIST(INK)			
2.	00103	DIMENSION AXES(5,6),TITLE(7,6),TITL(7)			*NEW
3.	00104	DATA AXES/ 0.,0.,10.,0.,1., -5., 5., 7., 2.4.,2,			*NEW
4.	00104	1 0., 0.,12.,.2.,.05, 10.,0.,12.,0.,.02,			*NEW
5.	00104	2 10.5, 0., 12.,0.,.25, 10.,0.,12.,0.,.25 /			*NEW
6.	00106	DATA TITLE/			*NEW
7.	00106	142H BURNUP (UNITS: GWD/MTM)			*NEW
8.	00106	242H PU-239 (UNITS: .0001 ATOMS/B-CM)			*NEW
9.	00106	342H PU-240 (UNITS: .0001 ATOMS/B-CM)			*NEW
10.	00106	442H PU-241 (UNITS: .0001 ATOMS/B-CM)			*NEW
11.	00106	542H PU-242 (UNITS: .000001 ATOMS/B-CM)			*NEW
12.	00106	642HPU-239 FISSIONS (UNITS: .0001 ATOMS/B-CM) /			*NEW
13.	00110	DATA TITL/42H U-235 (UNITS: .0001 ATOMS/B-CM) /			*NEW
14.	00112	J1=5			*NEW
15.	00113	IF(ND.EQ.0) GO TO 100			*NEW
16.	00115	DO 50 I=1,7			*NEW
17.	00120	50 TITLE(I,1)=TITL(I)			*NEW
18.	00122	AXES(3,1)=9.			*NEW

19.	00123	AXES(4,1)=1.5	*NEW
20.	00124	AXES(5,1)=-.05	*NEW
21.	00125	AXES(1,4)=9.	*NEW
22.	00126	AXES(1,5)=9.5	*NEW
23.	00127	AXES(1,6)=10.5	*NEW
24.	00127	C DO (TICS SCALES TAGS) /XIS(X,Y,TAG,NH,SPAN,ANGLE,DATA1,DATA/INCH)	*NEW
25.	00130	100 DO 200 J=1,J1	*NEW
26.	00133	LABEL=-42	*NEW
27.	00134	IF(J,LQ.2.OR.J.EQ.3) LABEL=42	*NEW
28.	00136	ANGLE=90.	*NEW
29.	00137	IF(J,LQ.1) ANGLE=0.	*NEW
30.	00141	200 CALL AXIS(AXES(1,J),AXES(2,J),TITLE(1,J),LABEL,AXES(3,J),ANGLE,AXE	*NEW
31.	00141	1S(4,J),AXES(5,J))	*NEW
32.	00143	ND=1	*NEW
33.	00144	RETURN	
34.	00145	END	

TABLE VI (Cont'd.)

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END OF UNIVAC 1108 FORTRAN V COMPILATION. 0 *DIAGNOSTIC* MESSAGE(S)

PHASE 1 TIME = 0 SEC.
 PHASE 2 TIME = 0 SEC.
 PHASE 3 TIME = 0 SEC.
 PHASE 4 TIME = 0 SEC.
 PHASE 5 TIME = 0 SEC.
 PHASE 6 TIME = 0 SEC.

TOTAL COMPILATION TIME = 1 SEC
 ARTIST SYMBOLIC
 ARTIST CODE RELOCATABLE

02 APR 68	12:27:54	0	00440214	14	3 (DELETED)
02 APR 68	12:27:54	1	00440114	36	1 (DELETED)
		0	00440160	14	2

MSG 300 PAPER FLUID INK PEN

SYS

* MSG LABEL TAPE H. PLOT TAPE H ON CALCOMP

SYS

* MSG R P MATSEN CUS114 ROB BLDG 3000 AREA

SYS

*N XQT.U DBUFIT

THIS ALLOCATION WAS DONE ON 31 MAR 70 AT 11:56:58

SYS

TABLE VI (Cont'd.)

MAXIMUM LIKELIHOOD NONLINEAR CORRELATED FIELDS
PROGRAM DBUFIT(01SEP69) A MODIFIED, DOUBLE PRECISION VERSION OF
BATTELLE-NORTHWEST PROGRAM LIKELY (05SEP65) BNWL-284
FOR DERIVING CROSS SECTION RATIOS FROM ISOTOPIC CONCENTRATION DATA

ITERATE LIMIT	X-COORDINATES	Y-COORDINATES	P-COORDINATES	Q-COORDINATES	MEASUREMENTS		
IL 25	IX 1	JY 6	KP 13	LQ 5	MM 9		
UGEN(ERATOR)	UEXP(ONENT)	YEXP(ONENT)	Q EQUATIONS	FIXED PARAM	CONTROL CONSTANTS	BAD (REFIT)	
-0.0000000	-0.0000000	-0.0000000	JUMPED 0	N 2	LIKCON 0100101200	3.0000000+00	
CONSTANTS C(N),N=1, 9							
0.0000000	2.2300000+01	2.1287000+02	2.2232000+02	2.2514000+02	1.1100000+00	3.0000000-02	2.1970000-01
9.0000000-04							

TABLE VI (Cont'd.)

TABLE VI (Cont'd.)

PARAMETER ESTIMATES P(I) I=1, 20							
2.046780000000000+002	1.604132678619039-002	-1.500000000000000+000	2.000000000000000+000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000
3.790999978780746+000	1.500000000000000+000	0.000000000000000	1.400000000000000+000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000
3.445999994874000-001	2.500000000000000+000	4.770093977031350-002	4.258499999999999+000	3.332299995236098-003			
4.101999999999999-001	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000

PARAMETER-VARIATION DELAY LAG(K), K=1, 20															
0	0	0	0	0	0	0	0	0	0	0	0	0	0	99	0

MEASUREMENT VECTORS ((IMPRECISE Y(M,J), J=1, 6), (PRECISE X(M,I), I=1, 1)), M=1, 9

	M= 1	M= 2	M= 3	M= 4	M= 5	M= 6	M= 7
Y(M, 1)=	1.4851000+00	1.4056000+00	1.824000+00	1.3557000+00	1.3058000+00	1.2690000+00	1.2376000+00
Y(M, 2)=	3.7910000+00	3.4604000+00	3.4692000+00	3.3290000+00	3.2066000+00	3.1518000+00	3.0038000+00
Y(M, 3)=	0.0000000	2.4449000-01	3.4452000-01	4.7442000-01	6.4315999-01	7.4722999-01	8.5647000-01
Y(M, 4)=	3.4460000-01	4.3324000-01	4.7529000-01	5.0900000-01	5.7653999-01	6.1460999-01	6.4613000-01
Y(M, 5)=	4.7701000-02	7.0961999-02	8.4475999-02	9.7208999-02	1.1730000-01	1.3040000-01	1.3863000-01
Y(M, 6)=	3.3323000-03	5.0175999-03	6.0017999-03	7.2904000-03	9.8666999-03	1.1567000-02	1.3619000-02
X(M, 1)=	0.0000000	1.5443000+03	2.1381000+03	2.9037000+03	3.9614000+03	4.6471000+03	5.3380000+03
	M= 8	M= 9					
Y(M, 1)=	119.0000+00	1.119000+00					
Y(M, 2)=	2.841000+00	2.676500+00					
Y(M, 3)=	1.063000+00	1.2180100+00					
Y(M, 4)=	6.990000-01	7.770000-01					
Y(M, 5)=	1.625000-01	1.962800-01					
Y(M, 6)=	1.780999-02	2.5164700-02					
X(M, 1)=	6.585999+03	8.048300+03					

MEAN SQUARE CORRELATED-MEASUREMENT-UNCERTAINTY TENSORS ((U(M,J1,J2),J1=1, 6),J2=1, 6),M=1, 9														
	J2= 1	1=M	J2= 2	1=M	J2= 3	1=M	J2= 4	1=M	J2= 5	1=M	J2= 6	1=M	J2= 1	2=M
U(M, 1,J2)=	2.2000000-00		0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		8.1199999-00	

U(M, 2,J2)=	0.0000000	1.4396000-03	0.0000000	1.2820000-04	1.8050000-05	1.2600000-06	0.0000000
U(M, 3,J2)=	0.0000000	0.0000000	9.9999997-21	0.0000000	0.0000000	0.0000000	0.0000000
U(M, 4,J2)=	0.0000000	1.2820000-04	0.0000000	1.4300000-05	3.6080000-06	1.1230000-07	0.0000000
U(M, 5,J2)=	0.0000000	1.8050000-05	0.0000000	1.6080000-06	2.9600000-07	1.5800000-08	0.0000000
U(M, 6,J2)=	0.0000000	1.2600000-06	0.0000000	1.1230000-07	1.5800000-08	6.7149999-09	0.0000000

	J2= 2	2=M	J2= 3	2=M	J2= 4	2=M	J2= 5	2=M	J2= 6	2=M	J2= 1	3=M	J2= 2	3=M	
U(M, 1,J2)=	0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		3.0978999-06		0.0000000		TABLE VI (Cont'd.)
U(M, 2,J2)=	3.6403999-03		0.0000000		4.5578000-04		7.1651999-05		5.2839999-06		0.0000000		3.5309000-03		
U(M, 3,J2)=	0.0000000		7.1231999-05		0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		
U(M, 4,J2)=	4.5578000-04		0.0000000		5.8979999-05		9.3766993-06		0.0130000-07		0.0000000		4.8373000-04		
U(M, 5,J2)=	7.4653999-05		0.0000000		9.3466999-06		1.6053000-06		1.0832000-07		0.0000000		8.5976999-05		
U(M, 6,J2)=	5.2819999-05		0.0000000		6.6130999-07		1.0332000-07		1.2454000-08		0.0000000		6.1122999-06		

	J2= 3	3=M	J2= 4	3=M	J2= 5	3=M	J2= 6	3=M	J2= 1	4=M	J2= 2	4=M	J2= 3	4=M	
U(M, 1,J2)=	0.0000000		0.0000000		0.0000000		0.0000000		9.6431998-06		0.0000000		0.0000000		
U(M, 2,J2)=	0.0000000		4.8373000-04		8.5976993-05		6.1122999-06		0.0000000		3.5537000-03		0.0000000		
U(M, 3,J2)=	8.4050000-05		0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		1.7275000-04		
U(M, 4,J2)=	0.0000000		6.8106999-05		1.1779000-05		8.3738999-07		0.0000000		5.1278000-04		0.0000000		
U(M, 5,J2)=	0.0000000		1.1779000-05		2.2880000-06		1.4884000-07		0.0000000		9.7931998-05		0.0000000		
U(M, 6,J2)=	0.0000000		8.3738999-07		1.4884000-07		1.5395000-08		0.0000000		7.3476999-06		0.0000000		

	J2= 4	4=M	J2= 5	4=M	J2= 6	4=M	J2= 1	5=M	J2= 2	5=M	J2= 3	5=M	J2= 4	5=M	
U(M, 1,J2)=	0.0000000		0.0000000		0.0000000		9.6293999-06		0.0000000		0.0000000		0.0000000		35
U(M, 2,J2)=	5.1218000-04		9.7931998-05		7.3476999-06		0.0000000		2.0008000-03		0.0000000		5.1076999-04		
U(M, 3,J2)=	0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		2.1290000-04		0.0000000		
U(M, 4,J2)=	8.1174999-05		1.4974000-05		1.1235000-06		0.0000000		5.3076999-04		0.0000000		1.0017000-04		
U(M, 5,J2)=	1.4974000-05		3.1037000-06		2.1455999-07		0.0000000		1.0391000-04		0.0000000		1.8684000-05		
U(M, 6,J2)=	1.1235000-06		2.1455999-07		2.0570999-08		0.0000000		8.7483999-06		0.0000000		1.5730000-06		

	J2= 5	5=M	J2= 0	5=M	J2= 1	0=M	J2= 2	6=M	J2= 3	6=M	J2= 4	6=M	J2= 5	6=M	
U(M, 1,J2)=	0.0000000		0.0000000		9.0101998-06		0.0000000		0.0000000		0.0000000		0.0000000		
U(M, 2,J2)=	1.0391000-04		8.7483999-06		0.0000000		2.7430000-03		0.0000000		5.3488999-04		1.1348000-04		
U(M, 3,J2)=	0.0000000		0.0000000		0.0000000		0.0000000		2.9737000-04		0.0000000		0.0000000		
U(M, 4,J2)=	1.8684000-05		1.5700000-06		0.0000000		5.3488999-04		0.0000000		1.1424000-04		2.2129000-05		
U(M, 5,J2)=	4.2839999-06		3.2001000-07		0.0000000		1.1348000-04		0.0000000		2.2129000-05		5.1205000-06		
U(M, 6,J2)=	3.2001000-07		3.0811999-08		0.0000000		1.0072000-05		0.0000000		1.9640999-06		4.1671000-07		

	J2= 6	6=M	J2= 1	7=M	J2= 2	7=M	J2= 3	7=M	J2= 4	7=M	J2= 5	7=M	J2= 6	7=M	
U(M, 1,J2)=	0.0000000		9.6179000-06		0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		
U(M, 2,J2)=	1.0072000-05		0.0000000		2.4851999-03		0.0000000		5.3455999-04		1.1469000-04		1.1279000-05		
U(M, 3,J2)=	0.0000000		0.0000000		0.0000000		3.5598000-04		0.0000000		0.0000000		0.0000000		
U(M, 4,J2)=	1.9640999-06		0.0000000		5.3455999-04		0.0000000		1.2590000-04		2.4670000-05		2.4262000-06		
U(M, 5,J2)=	4.1671000-07		0.0000000		1.1469000-04		0.0000000		2.4670000-05		5.7860999-06		5.2053998-07		
U(M, 6,J2)=	4.4774000-08		0.0000000		1.1279000-05		0.0000000		2.4262000-06		5.2053998-07		6.9463999-08		

	J2= 1	8=M	J2= 2	8=M	J2= 3	8=M	J2= 4	8=M	J2= 5	8=M	J2= 6	8=M	J2= 1	9=M	
U(M, 1,J2)=	9.6039999-06		0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		8.0547998-06		
U(M, 2,J2)=	0.0000000		2.2387000-03		0.0000000		5.4961000-04		1.2746000-04		1.4076000-05		0.0000000		

U(F, 3,J2)=	0.0000000	0.0000000	5.1102000-04	0.0000000	0.0000000	0.0000000	0.0000000
U(F, 4,J2)=	0.0000000	5.4961000-04	0.0000000	1.4661000-04	3.1291000-05	3.4557000-06	0.0000000
U(F, 5,J2)=	0.0000000	1.2746000-04	0.0000000	3.1291000-05	7.9242998-06	8.0138998-07	0.0000000
U(F, 6,J2)=	0.0000000	1.4076000-05	0.0000000	3.4557000-06	8.0138998-07	1.0642000-07	0.0000000

	J2= 2	9=M	J2= 3	9=M	J2= 4	9=M	J2= 5	9	J2= 6	9=M	
U(M, 1,J2)=	0.0000000		0.0000000		0.0000000		0.0000000		0.0000000		
U(M, 2,J2)=	1.9737000-03		0.0000000		5.7207999-04		1.4474000-04		1.8492000-05		
U(M, 3,J2)=	0.0000000		7.4608999-04		0.0000000		0.0000000		0.0000000		
U(M, 4,J2)=	5.7297999-04		0.0000000		1.8245000-04		4.2017999-05		5.3681999-06		
U(M, 5,J2)=	1.4474000-04		0.0000000		4.2017999-05		1.1605000-05		1.3561000-06		
U(M, 6,J2)=	1.8492000-05		0.0000000		5.3681999-06		1.3561000-06		2.0835000-07		

TABLE VI (Cont'd.)

SUM OF UNCERTAINTY ELEMENTS
3.3146371-02
TIME=.7910-00ECONOS

NEXT MOVE TRY TAG	PARAMETER *	MISEIT	MISEIT GRADIENT	MISEIT 2ND GRAD	MATRIX INVERSION	NEXT MOVE	NEXT TREND
TYPE IT K	P(K) PIN	QQ=SUM(QQ(M))	DQQ/DP(K)	DDQQ/DP(K)/DP(K)	BLADE PIVOTS	DP(K)	DQQ=(DQQ/DP)DP/2
1 3	-1.5000000+00		-9.3383037+02	2.2494251+03	-1.1381715+02	7.2359039-01	
1 4	2.0000000+00		9.8994730+01	1.2737947+04	8.1670759+03	3.6825402-01	
1 5	0.0000000		-4.9445239+02	1.7937177+04	3.8845442+02	-4.4844174-01	
1 6	3.7910000+00		1.9192702+03	2.3478178+04	5.0402987+03	2.7550324-02	
1 7	1.5000000+00		-2.2824455+01	6.5198016+04	2.8544798+04	-2.4434809-01	
1 8	0.0000000		2.3348542+03	5.4241730+05	1.8871846+05	-7.9834934-03	
1 9	1.4000000+00		-3.5526335+03	8.9637870+04	8.2055566+03	-6.4377510-02	
1 10	0.0000000		-1.3580131+04	7.0265966+05	5.0349738+05	5.3253818-02	
1 11	3.4460000-01		4.7780549+03	1.8498731+06	1.6401033+06	-8.0613580-03	
1 12	2.5000000+00		-1.3575739+03	1.6169137+04	4.5342886+03	2.1263260-01	
1 13	4.7701000-02		-1.2696403+05	4.6534672+07	4.6023517+07	9.6521208-04	
1 14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX 1 15	3.3323000-03	1.0450315+03	-3.2595608+05	1.8732245 09	1.8732245+09	-1.8153615-04	-6.3137481+02
TIME=.4843+01SECONDS							
2 3	-7.7640960-01		1.9495492+02	2.2239933+03	2.5176817+02	-6.7032661-01	
2 4	2.3682540+00		-4.4303925+02	7.9000603+03	4.6443066+03	-1.1434221-01	
2 5	-4.4844174-01		6.2851410+01	2.2265676+04	5.0917052+02	3.7303428-01	
2 6	3.8185503+00		-4.0543432+02	2.2508282+04	5.4416449+03	-8.4774514-02	
2 7	1.2556519+00		-1.2012649+03	8.8360898+04	3.5592898+04	2.9505910-02	
2 8	-7.9834934-03		-2.0184835+03	5.8020674+05	1.8098942+05	-4.0281328-03	
2 9	1.3356225+00		-3.3810548+02	8.9505884+04	2.3036631+03	-2.2613754-01	
2 10	5.3253818-02		-2.6512329+03	5.5529459+05	3.7973687+05	1.3631754-01	
2 11	3.3653864-01		2.6287958+03	1.8617511+06	1.5823488+06	-8.5732360-03	
2 12	2.7126326+00		-3.9436856+02	1.3179597+04	3.4638196+03	1.6240425-01	
2 13	4.8666212-02		-9.5494060+03	4.5781936+07	4.5395949+07	-2.2633013-03	
2 14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX 2 15	3.1507638-03	4.1416402+02	-7.5018093+04	1.8379296+09	1.8379296+09	-9.1637246-05	-1.9628541+02
TIME=.8928+01SECONDS							
3 3	-1.4467362+00		-8.0719580+01	2.2433175+03	4.4517493+02	2.7499577-01	
3 4	2.2539118+00		8.2715286+01	1.0074680+04	6.3397077+03	1.8952569-01	
3 5	-7.5407466-02		1.1688825+03	2.0837361+04	7.1712362+01	-3.0684498-01	
3 6	3.7337758+00		5.9494828+02	2.3601951+04	4.7019357+03	2.0134924-02	
3 7	1.2851578+00		-3.0656186+03	1.0781495+05	4.4320851+04	-8.8706326-02	
3 8	-1.2011626-02		5.1479566+02	5.9711745+05	1.7065683+05	1.5545679-03	
3 9	1.1094449+00		-6.7337243+03	1.5673686+05	1.4278899+04	-1.7587278-02	
3 10	1.8957137-01		-1.1571445+04	4.0873213+05	2.7441231+05	5.6656620-03	
3 11	3.2796541-01		7.8144382+03	1.9639564+06	1.6464547+06	2.5961905-03	
3 12	2.8750368+00		8.3106607+02	1.2605215+04	2.9513447+03	-4.6048074-02	
3 13	4.6402910-02		-5.7611715+04	4.5860611+07	4.5350973+07	5.1458061-04	
3 14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MAT/2 3 15	3.0591266-03	3.2295459+02	1.2552319+04	1.8268346+09	1.8268346+09	4.0366879-05	-1.2755158+02
TIME=.1307+02SECONDS							

TABLE VI (Cont'd.)

37

	4	3	-1.1717404+00		-3.3485010+01	2.4776781+03	4.4043137+02	-2.2010130-01	TABLE VI (Cont'd.)
	4	4	2.4434375+00		-9.4284484+01	8.1134041+03	4.5081186+03	-1.9256615-01	
	4	5	-3.8225245-01		6.4357378+02	2.4211399+04	1.3331611+02	2.6750275-01	
	4	6	3.7539107+00		2.6601031+02	2.3431113+04	5.3677324+03	-9.2693595-03	
	4	7	1.1964515+00		-2.0590954+03	1.1774292+05	4.6777106+04	8.2466725-02	
	4	8	-1.0457058-02		-1.3112393+02	5.9969992+05	1.7203262+05	-1.8864255-03	
	4	9	1.0918977+00		-4.5082942+03	1.5590289+05	1.0409940+04	7.0209248-03	
	4	10	1.9523703-01		-7.8398371+03	3.9180014+05	2.6199631+05	1.4335473-02	
	4	11	3.3056159-01		5.2528995+03	1.9882859+06	1.6613681+06	-1.3054330-03	
	4	12	2.8289888+00		6.1749976+02	1.2757397+04	2.9681002+03	3.6353765-02	
	4	13	4.6917491-02		-3.7870093+04	4.5822255+07	4.5381138+07	-4.8494409-04	
	4	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MAT/2	4	15	3.0994935-03	2.6435161+02	2.4089351+04	1.8261199+09	1.8261199+09	-2.7057998-05	-1.4523278+02

TIME=.1720+02SECONDS

	5	3	-1.3918417+00		-1.7600804+01	2.1829084+03	3.5694531+02	-3.1283429-01	38
	5	4	2.2508714+00		-2.2841728+02	9.9107359+03	6.2040664+03	-2.5717712-01	
	5	5	-1.1474969-01		3.1959157+02	2.1483482+04	1.5580077+02	4.4166957-01	
	5	6	3.7446413+00		8.7122912+01	2.3264690+04	4.9010488+03	-4.1910260-03	
	5	7	1.2789182+00		-1.4079257+03	1.0643609+05	4.1410071+04	1.4858227-01	
	5	8	-1.2343484-02		-5.5628637+02	6.2682832+05	1.7429594+05	-1.1360553-03	
	5	9	1.0989186+00		-2.9225007+03	1.6002838+05	7.4403687+03	-2.6075011-02	
	5	10	2.0957250-01		-5.1560027+03	3.9096566+05	2.5858633+05	4.3162616-02	
	5	11	3.2925616-01		3.4308964+03	1.9831365+06	1.6524924+06	3.1670262-04	
	5	12	2.8653426+00		4.6736238+02	1.2846458+04	2.8732374+03	2.5461177-02	
	5	13	4.6432547-02		-2.3830236+04	4.5536695+07	4.5080744+07	-4.6926685-04	
	5	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	5	15	3.0724355-03	1.9335818+02	3.1871306+04	1.8229623+09	1.8229623+09	-7.2998760-06	-6.2964165+01

TIME=.2129+02SECONDS

	6	3	-1.7046760+00		3.5903015+00	1.8185265+03	2.3743396+02	4.5987297-02	
	6	4	1.9936942+00		-3.7431748+02	1.3045739+04	8.1821608+03	-1.1400010-02	
	6	5	3.2691987-01		-1.7857262+02	1.7809459+04	1.4319339+02	1.2970245-02	
	6	6	3.7404504+00		-1.5009449+02	2.3451748+04	5.0502048+03	1.3934639-02	
	6	7	1.4275005+00		-1.6015311+02	8.7716593+04	3.2519602+04	2.1149140-02	
	6	8	-1.3479539-02		-9.7252305+02	6.6656280+05	1.7556188+05	1.1904155-03	
	6	9	1.0728436+00		3.0333998+02	1.7612274+05	1.0340605+03	-8.7830396-02	
	6	10	2.5273512-01		4.0477920+01	3.6474143+05	2.3621770+05	5.6772214-02	
	6	11	3.2957286-01		-1.7302758+02	2.0099235+06	1.6632532+06	3.1196588-03	
	6	12	2.8908037+00		9.3722869+01	1.3035941+04	2.9678841+03	-3.1035776-02	
	6	13	4.5963280-02		2.6944673+03	4.5192361+07	4.4757718+07	1.1816671-04	
	6	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MAT/2	6	15	3.0651356-03	1.2453664+02	2.8050477+04	1.8190720+09	1.8190720+09	3.8994943-05	-5.2749824+01

TIME=.2542+02SECONDS

	7	3	-1.6586887+00		-4.0485330+00	1.8341173+03	2.6665734+02	-4.4461753-02	
	7	4	1.9822642+00		-2.3246120+02	1.3076762+04	8.3403941+03	-1.0310989-01	
	7	5	3.3989011-01		9.3332035+01	1.7504733+04	9.7969467+01	2.0502970-01	
	7	6	3.7543550+00		-1.2151493+01	2.3813204+04	5.0648165+03	0.9393552-03	
	7	7	1.4486496+00		-6.3882442+02	8.5789026+04	3.1835075+04	0.8221649-02	
	7	8	-1.2289124-02		-5.4699371+02	6.6909663+05	1.7403764+05	2.0135587-03	
	7	9	9.8501318-01		-1.1371844+03	2.1246323+05	4.1057838+03	-4.9768077-02	
	7	10	3.0950733-01		-1.6332091+03	3.1759395+05	2.0465211+05	4.0864063-02	
	7	11	3.3269253-01		1.6928070+03	2.0666332+06	1.7022593+06	3.1678112-03	
	7	12	2.8597880+00		1.8551099+02	1.3106818+04	2.8346034+03	2.3079374-02	
	7	13	4.6081447-02		-8.3953355+03	4.5380468+07	4.4964687+07	2.225951-04	
	7	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	7	15	3.1041506-03	1.0253904+02	1.9155353+04	1.8209175+09	1.8209175+09	2.3185761-05	-1.5592298+01
					TIME=.2944+02SECONDS				
	8	3	-1.7031505+00		4.4303880+00	1.7104972+03	2.2970676+02	-1.0299605-01	
	8	4	1.8791043+00		-5.6630187+01	1.4444693+04	9.3659092+03	-1.4635763-01	
	8	5	5.4491981-01		8.7088774+01	1.5754141+04	3.8680911+01	2.9372454-01	
	8	6	3.7643043-00		2.4343874-01	2.4281496+04	5.1046037+03	5.7473324-03	
	8	7	1.5468713+00		-3.2930716+02	7.4018041+04	2.7059672+04	1.3119390-01	
	8	8	-1.0275565-02		-1.5440077+02	6.7075000+05	1.7201204+05	1.5220237-03	
	8	9	9.3524431-01		-5.5956069+02	2.3685616+05	2.5938716+03	-4.4268078-02	
	8	10	3.5037149-01		-7.7280600+02	2.8886513+05	1.8518019+05	3.9460777-02	
	8	11	3.3586033-01		1.0150192+03	2.1108019+06	1.7320443+06	2.5721091-03	
	8	12	2.8368885+00		5.3397189+01	1.3181345+04	3.0689115+03	1.3850865-02	
	8	13	4.6305706-02		-4.3021667+03	4.5458519+07	4.5075192+07	9.30042594-05	
	8	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	8	15	3.1273163-03	8.2602464+01	-2.8181987+02	1.8212792+09	1.8212792+09	1.3213040-05	-7.1489183+00
					TIME=.3351+02SECONDS				
	9	3	-1.8061765+00		6.3684945+00	1.5244554+03	1.9906469+02	-1.2364091-02	
	9	4	1.7328267+00		-1.6064544+02	1.6947682+04	1.1443705+04	-3.2617819-02	
	9	5	8.3864036-01		4.1791753+01	1.3700325+04	4.5437232+01	9.2122831-02	
	9	6	3.7700716+00		-3.9063803+01	2.4793446+04	5.2119473+03	3.7714035-03	
	9	7	1.6780652+00		-2.8345740+02	6.2600655+04	2.2840747+04	4.7465254-02	
	9	8	-8.7535413-03		-3.3836858+02	6.8878742+05	1.7537934+05	5.5507453-04	
	9	9	8.9097623-01		-5.0334200+02	2.6430305+05	1.7976299+05	-2.7415494-02	
	9	10	3.8983227-01		-5.7273556+02	2.6632560+05	2.3585553+03	2.6781876-02	
	9	11	3.3843245-01		9.7718660+02	2.1451007+06	1.7537544+06	1.2259892-03	
	9	12	2.8228378+00		6.2178499+01	1.3284003+04	2.8774075+03	-1.0139523-02	
	9	13	4.6402349-02		-3.0630193+03	4.5489991+07	4.5119826+07	5.3719155-05	
	9	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	9	15	3.1405799-03	7.4371936+01	4.6630118+03	1.8207280+09	1.8207280+09	9.8107664-06	-2.9345874+00
					TIME=.3758+02SECONDS				

TABLE VI (Cont'd.)

	10	3	-1.8188106+00		7.6153944-01	1.4898783+03	1.8299883+02	-5.2524200-02	TABLE VI (Cont'd.)
	10	4	1.7002089+00		-4.3985741+00	1.7565824+04	1.1902174+04	-5.8003737-02	
	10	5	9.3076719-01		3.0835513+01	1.3190468+04	1.2105857+01	1.4028389-01	
	10	6	3.7738431+00		5.2930171+00	2.5080509+04	5.2159754+03	1.1461834-03	
	10	7	1.7255304+00		-8.9258178+01	5.8666548+04	2.1140634+04	6.1972331-02	
	10	8	-8.184067-03		-1.4643731+01	6.8505564+05	1.7306882+05	5.5126251-04	
	10	9	8.656073-01		-2.2490731+02	2.8178796+05	1.9051186+05	-1.5150767-02	
	10	10	4.1661415-01		-2.4659868+02	2.5148959+05	1.4934310+03	1.5863675-02	
	10	11	3.3965443-01		3.3903676+02	2.1707387+06	1.7720740+06	8.7678726-04	
	10	12	2.8126982+00		1.8184456+01	1.3287093+04	2.8569736+03	-4.5347476-03	
	10	13	4.6456068-02		-1.5463393+03	4.5516254+07	4.5159210+07	2.6109856-05	
	10	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	10	15	3.1503407-03	7.0884965+01	-2.9282968+02	1.8208332+09	1.8208332+09	3.6788628-06	-6.6188833-01
TIME=.4164+02SECONDS									
	11	3	-1.8710349+00		9.8627853-01	1.4154766+03	1.6812271+02	1.4530963-02	10
	11	4	1.6422051+00		-3.3345120+01	1.8827642+04	1.2851797+04	4.9516246-03	
	11	5	1.0710511+00		3.1781474+00	1.2430960+04	1.2992657+01	-1.0951256-02	
	11	6	3.7749892+00		-8.7298758+00	2.5335333+04	5.2439168+03	1.5810360-03	
	11	7	1.7875028+00		-3.9006978+01	5.4521941+04	1.9556946+04	-1.7171647-03	
	11	8	-7.6472043-03		-6.4960467+01	6.9144674+05	1.7398333+05	2.0336605-05	
	11	9	8.4840997-01		-7.0708324+01	2.9320592+05	1.9768303+05	-9.0521587-03	
	11	10	4.3247782-01		-7.2706325+01	2.4390540+05	1.0546695+03	9.5312766-03	
	11	11	3.4053522-01		1.4451944+02	2.1839927+06	1.7807429+06	2.7557731-04	
	11	12	2.8081835+00		9.9618582+00	1.3321976+04	2.8610709+03	-3.0385343-03	
	11	13	4.6482178-02		3.7147615+02	4.5520867+07	4.5168993+07	9.1546208-06	
	11	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	11	15	3.1540196-03	7.0160887+01	1.0459003+03	1.8205696+09	1.8205696+09	3.6074116-06	-8.8359786-02
TIME=.4570+02SECONDS									
	12	3	-1.8565039+00		4.1089821-02	1.4238764+03	1.6671491+02	1.4603050-02	
	12	4	1.6471567+00		4.2253127-01	1.8090666+04	1.2756919+04	9.5488519-03	
	12	5	1.0600998+00		3.1106804+00	1.2476022+04	6.6651960+00	-2.5712349-02	
	12	6	3.7765703+00		1.0174171+00	2.5356974+04	5.2387482+03	7.6974117-04	
	12	7	1.7857856+00		-7.2477879+00	5.4566120+04	1.9500063+04	-9.9298680-03	
	12	8	-7.6268077-03		1.3999881-00	6.9064413+05	1.7338104+05	-7.6281194-05	
	12	9	8.3935781-01		-2.6156153+01	2.9976396+05	2.0165471+05	-3.4251423-03	
	12	10	4.4200910-01		-2.4965023+00	2.3914859+05	9.1396293+02	3.7993513-03	
	12	11	3.4081080-01		0.3168715+00	2.1919186+06	1.7863512+06	3.8450579-05	
	12	12	2.8051249+00		2.1392482+00	1.3323384+04	2.8592213+03	-9.5395344-04	
	12	13	4.6491332-02		-1.6856924+00	4.5527185+07	4.5178739+07	-1.4753686-06	
	12	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	12	15	3.1576270-03	7.0065953+01	2.2242706+00	1.8206289+09	1.8206289+09	1.5394201-06	-4.8235513-03
TIME=.4915+02SECONDS									
	13	3	-1.8419009+00		2.5778417-02	1.4367337+03	1.6766723+02	1.0758653-03	

	13	4	1.6567056+00		-9.1058657-01	1.8460081+04	1.2590938+04	7.5771003-04	
	13	5	1.0343875+00		1.6451840-01	1.2609100+04	6.8098807+00	-1.8675875-03	
	13	6	3.7773400+00		-2.4423299-01	2.5323787+04	5.2345648+03	7.2051256-05	
	13	7	1.7758557+00		-1.2541339+00	5.5207866+04	1.9698680+04	-7.2063005-04	
	13	8	-7.7031489-03		-1.8306565+00	6.9085348+05	1.7327447+05	-7.6426814-06	
	13	9	8.3593266-01		-3.4172473+00	3.0235815+05	2.0319145+05	-3.7293618-04	
	13	10	4.4580845-01		-3.2286571+00	2.3732134+05	8.5394912+02	4.2856421-04	
	13	11	3.4084925-01		5.4327579+00	2.1946549+06	1.7882065+06	4.5311339-06	
	13	12	2.8041709+00		4.4885933-01	1.3325988+04	2.8596606+03	-8.9159807-05	
	13	13	4.6489857-02		-1.8327261+01	4.5526432+07	4.5179088+07	-3.8102114-07	
	13	14	4.2585000+00*		0.0000000	0.0000000	0.0000000	0.0000000	
MATRIX	13	15	3.1591064-03	7.0060839+01	4.8136415+01	1.8206324+09	1.8206324+09	1.4966940-07	-8.9903148-05
					TIME=-.5382+02SECONDS				

TABLE VI (Cont'd)

MAXIMUM-LIKELIHOOD STATISTICAL ANALYSIS

TAG	BEST FIT PARAMETER	* PIN	ROOT MEAN SQUARE DOUBT DP(K)	MEASUREMENT VARIANCE I*I=-1 QQ/(MM*LQ-KP)	MISFIT GRADIENT DQQ/DP(K) SHOULD BE 0	MISFIT 2ND GRAD DDQQ/DP(K)/DP(K) SHOULD BE POSITIVE	MATRIX INVERSION BLADE PIVOTS MINUS=SADDLE	MATRIX STEP DP(K) PREDICTED
K	P(K)							
3	-1.8408250+00		4.5686176-01		7.1412285-05	1.4377808+03	1.6766839+02	4.5517339-05
4	1.6574633+00		3.0412797-01		-4.9412528-03	1.8442297+04	1.2577812+04	3.1759439-05
5	1.0325199+00		8.0115960-01		4.1500059-03	1.2619036+04	6.6153486+00	-8.3142035-05
6	3.7774121+00		4.3957271-02		-2.4259550-04	2.5321971+04	5.2341634+03	2.2581462-06
7	1.7751351+00		3.1930627-01		-1.4166551-02	5.5255475+04	1.9712012+04	-3.2618299-05
8	-7.7107915-03		6.9805292-03		-8.6488426-03	6.9084021+05	1.7324967+05	-2.6833254-07
9	8.3555973-01		9.0304498-02		-4.5917185-02	3.0264688+05	2.0336250+05	-9.7010291-06
10	4.4623701-01		9.8643830-02		-4.3640354-02	2.3712028+05	8.4572148+02	1.0832863-05
11	3.4085378-01		5.2403243-03		6.3974025-02	2.1949696+06	1.7884252+06	6.6092025-08
12	2.8040818+00		4.9013219-02		4.7135245-03	1.3326123+04	2.8595269+03	-2.5979108-06
13	4.6489476-02		9.4826505-04		-2.7384480-01	4.5526368+07	4.5179147+07	-7.6093222-09
14	4.2585000+00*		0.0000000		0.0000000	0.0000000	0.0000000	-0.0000000
15	3.1593161-03		8.7949460-05	2.1230530+00	2.8997556-01	1.8206339+09	1.8206339+09	4.4704220-09

TABLE VI (Cont'd.)

MEAN SQUARE CORRELATED PARAMETER ERROR (DPDP(K1,K2),K1= 3,15),K2= 3,15)

K1=	K2= 3	K2= 4	K2= 5	K2= 6	K2= 7	K2= 8	K2= 9
3	2.0872267-01	1.2689062-01	-3.4309676-01	1.2340251-02	-1.2983900-01	-7.8412952-04	-2.9968593-02
4	1.2689062-01	9.2493819-02	-2.4260659-01	5.1176689-03	-9.6755363-02	-7.6899233-04	-1.8639713-02
5	-3.4309676-01	-2.4260659-01	6.4185671-01	-1.4871319-02	2.5356571-01	1.7690187-03	5.0203026-02
6	1.2340251-02	5.1176689-03	-1.4871319-02	1.9322417-03	-5.0578484-03	-5.2580224-05	-1.7277153-03
7	-1.2983900-01	-9.6755363-02	2.5356571-01	-5.0578484-03	1.0195649-01	8.1456432-04	1.8940712-02
8	-7.8412952-04	-7.6899233-04	1.7690187-03	-5.2580224-05	8.1456432-04	4.8727788-05	1.3327948-04
9	-2.9968593-02	-1.8639713-02	5.0203026-02	-1.7277153-03	1.8940712-02	1.3327948-04	8.1549023-03
10	3.0807281-02	2.0437007-02	-5.4201305-02	1.7310436-03	-2.0996410-02	-1.9857309-04	-8.7980498-03
11	5.9126709-04	-6.6815882-05	-8.7100124-05	1.5181035-04	1.2842197-04	1.7728765-05	-1.2281722-04
12	-1.1884841-02	-5.1502322-03	1.5790614-02	-8.5725384-04	4.8813091-03	-9.0397530-05	2.4366548-03
13	6.9641249-05	-2.0335700-05	7.6552885-06	1.8374912-05	2.6957888-05	4.7164555-06	4.9585515-07
14	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
15	1.7753880-05	9.7108312-06	-2.7788346-05	1.6141981-06	-9.8532974-06	1.3759243-07	-3.6164470-06
K1=	K2= 10	K2= 11	K2= 12	K2= 13	K2= 14	K2= 15	
3	3.0807281-02	5.9126709-04	-1.1884841-02	6.9641249-05	0.0000000	1.7753880-05	
4	2.0437007-02	-6.6815882-05	-5.1502322-03	-2.0335700-05	0.0000000	9.7108312-06	
5	-5.4201305-02	-8.7100124-05	1.5790614-02	7.6552885-06	0.0000000	-2.7788346-05	
6	1.7310436-03	1.5181035-04	-8.5725384-04	1.8374912-05	0.0000000	1.6141981-06	
7	-2.0996410-02	1.2842197-04	4.8813091-03	2.6957888-05	0.0000000	-9.8532974-06	
8	-1.9857309-04	1.7728765-05	-9.0397530-05	4.7164555-06	0.0000000	1.3759243-07	
9	-8.7980498-03	-1.2281722-04	2.4366548-03	4.9585515-07	0.0000000	-3.6164470-06	

12

K1= 10	9.7306051-03	9.3016487-05	-2.1341480-03	-9.9655998-06	0.0000000	3.5296198-06
K1= 11	9.3016487-05	2.7461000-05	-1.3277918-04	3.8678065-00	0.0000000	2.2763924-07
K1= 12	-2.1341480-03	-1.3277918-04	2.4022956-03	-2.1430762-05	0.0000000	-3.0578407-06
K1= 13	-9.3655998-06	3.8678065-06	-2.1430762-05	8.9920662-07	0.0000000	3.4201449-08
K1= 14	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
K1= 15	3.3296198-00	2.2763924-07	-3.0578407-00	3.4201449-08	0.0000000	7.7351075-09

MEAN SQUARE CORRELATED ERROR PROPOGATES TO FUNCTION F HAVING PARAMETER GRADIENT F/DP AS DFD_F=(DF/DP).(DPPD).(DF/DP)

PARAMETER ERROR CORRELATION MATRIX

	K2= 3	K2= 4	K2= 5	K2= 6	K2= 7	K2= 8	K2= 9
K1= 3	1.0000000+00	9.1324721-01	-9.3737372-01	6.1448102-01	-8.9004695-01	-2.4587516-01	-7.2639387-01
K1= 4	9.1324721-01	1.0000000+00	-9.9569698-01	3.8281161-01	-9.9634844-01	-3.6222407-01	-6.7869316-01
K1= 5	-9.3737372-01	-9.9569698-01	1.0000000+00	-4.2227922-01	9.9120624-01	3.1631882-01	6.9390732-01
K1= 6	6.1448102-01	3.8281161-01	-4.2227922-01	1.0000000+00	-3.6035258-01	-1.7135759-01	-4.3524327-01
K1= 7	-8.9004695-01	-9.9634844-01	9.9120624-01	-3.6035258-01	1.0000000+00	3.6545137-01	6.5687007-01
K1= 8	-2.4587516-01	-3.6222407-01	3.1631882-01	-1.7135759-01	3.6545137-01	1.0000000+00	2.1142949-01
K1= 9	-7.2639387-01	-6.7869316-01	6.9390732-01	-4.3524327-01	6.5687007-01	2.1142949-01	1.0000000+00
K1= 10	6.8359461-01	6.8122569-01	-6.8583678-01	3.9921545-01	-6.6660363-01	-2.8837799-01	-9.8765918-01
K1= 11	2.4696803-01	-4.1924239-02	-2.0746344-02	6.5904106-01	7.6749174-02	4.8465418-01	-2.5953248-01
K1= 12	-5.3075651-01	-3.4550730-01	4.0213025-01	3.9789225-01	3.1190019-01	-2.6421349-01	5.5051784-01
K1= 13	1.6075037-01	-7.0513619-02	1.0076571-02	4.4082337-01	8.3032521-02	7.1252095-01	5.7904950-03
K1= 14	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
K1= 15	4.4185045-01	3.6305036-01	-3.9437599-01	4.1753507-01	-3.3086574-01	2.2411609-01	-4.5534392-01

	K2= 10	K2= 11	K2= 12	K2= 13	K2= 14	K2= 15
K1= 3	6.8359461-01	2.4696803-01	-5.3075651-01	1.6075037-01	0.0000000	4.4185045-01
K1= 4	6.8122569-01	-4.1924239-02	-3.4550730-01	-7.0513619-02	0.0000000	3.6305036-01
K1= 5	-6.8583678-01	-2.0746344-02	4.0213025-01	1.0076571-02	0.0000000	-3.9437599-01
K1= 6	3.9921545-01	6.5904106-01	-3.9789225-01	4.4082337-01	0.0000000	4.1753504-01
K1= 7	-6.6660363-01	7.6749174-02	3.1190019-01	8.9032521-02	0.0000000	-3.5086574-01
K1= 8	-2.8837799-01	4.8465418-01	-2.6421349-01	7.1252095-01	0.0000000	2.2411609-01
K1= 9	-9.8765918-01	-2.5953248-01	5.5051784-01	5.7904950-03	0.0000000	-4.5534392-01
K1= 10	1.0000000+00	1.7994171-01	-4.4140919-01	-1.0653781-01	0.0000000	4.0684111-01
K1= 11	1.7994171-01	1.0000000+00	-5.1696195-01	7.7835338-01	0.0000000	4.9391905-01
K1= 12	-4.4140919-01	-5.1696195-01	1.0000000+00	-4.6109949-01	0.0000000	-7.0936286-01
K1= 13	-1.0653781-01	7.7835338-01	-4.6109949-01	1.0000000+00	0.0000000	4.1009227-01
K1= 14	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
K1= 15	4.0684111-01	4.9391905-01	-7.0936286-01	4.1009227-01	0.0000000	1.0000000+00

TIME=.5831+02SECONDS

Table VI
(Cont'd.)

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ONE STANDARD DEVIATION ERRORS OF THE CROSS SECTION RATIOS ARE ENCLOSED IN PARENTHESES

ALPHA25 AB28/AB25 CAP28/AB25 CAP49/AB49 ALPHA49 AB41/AB25 CAP41/AB41 ALPHA41 LAM41/(PHI*AB41) AB42/AB25
 .2197(.0009) .01604 .01486(.00162) .3399(.0054) .5149(.0124) 2.5262(.0813) .2607(.0000) .3525(.0000) .110(.030) .41020

U235	PU238	AB49/AB25	PU240	AB40/AB25
.14851+01	.37774+01	2.111(.943)	.34085-00	1.929(.128)
.14394+01	.36272+01	2.129(.940)	.40282-00	1.761(.110)
.13937+01	.34801+01	2.149(.936)	.46244-00	1.642(.097)
.13480+01	.33360+01	2.170(.932)	.51970-00	1.553(.087)
.13023+01	.31951+01	2.193(.928)	.57454-00	1.485(.080)
.12567+01	.30573+01	2.217(.924)	.62694-00	1.430(.074)
.12110+01	.29227+01	2.243(.919)	.67685-00	1.386(.070)
.11653+01	.27913+01	2.271(.914)	.72424-00	1.350(.066)
.11196+01	.26633+01	2.300(.909)	.76906-00	1.320(.063)
.10739+01	.25385+01	2.332(.903)	.81126-00	1.295(.060)

TIME=.5840+02SECONDS

TABLE VI (Cont'd.)

2 HYPER-SPACE MAPS (Z-SCALES ((Z1,DZ,Z2)=(S1,DS,S2) INCHES), J=1,7))

DATA END POINT Z1	RESOLUTION DZ (0=DEPENDENT)	DATA END POINT Z2	PLOT END POINT S1	RESOLUTION DS (0=ORIGIN)	PLOT END POINT S2
1.5000000+00	-2.5000000-02	1.0500000+00	0.0000000	-5.0000000-01	8.0000000+00
4.0000001+00	0.0000000	1.4000000+00	1.3000000+01	0.0000000	0.0000000
0.0000000	0.0000000	3.2500000+00	0.0000000	0.0000000	1.3000000+01
2.0000000-01	0.0000000	8.4999999-01	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	2.6000000-01	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	3.2500000-02	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	1.0000000+04	0.0000000	1.0000000+00	1.0000000+01
1.5000000+00	-2.5000000-02	1.0500000+00	0.0000000	5.0000000-01	8.0000000+00
4.0000001+00	0.0000000	1.4000000+00	1.3000000+01	0.0000000	0.0000000
0.0000000	0.0000000	3.2500000+00	0.0000000	0.0000000	1.3000000+01
2.0000000-01	0.0000000	8.4999999-01	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	2.6000000-01	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	3.2500000-02	0.0000000	0.0000000	1.3000000+01
0.0000000	0.0000000	1.0000000+04	0.0000000	-1.0000000+00	1.0000000+01

TABLE VI (Cont'd.)

Z TRY OR DIE *	THEORY Y(Q(Y)=0)	I DOUBT DY	THEORY THEORY Q(Y) SHOULD BE 0	MEAN SQUARE MISS QWQ(Y)*	Z TRY OR DIE *	THEORY Y(Q(Y)=0)	I DOUBT DY	THEORY THEORY Q(Y) SHOULD BE 0	MEAN SQUARE MISS QWQ(Y)*
2=Pa2391	3.8270580+00	6.68629-02	-1.49625-09	1.62081-12	2	3.7439548+00	5.91587-02	-1.51922-08	1.09630-12
3=Pa2392	-6.0518537-02	1.12228-02	4.16703-11		3	2.8076843-02	9.16286-03	-1.97566-10	
4=Pa240	3.2014655-01	7.69337-03	-5.83263-09		4	3.5475463-01	7.12849-03	-4.97883-09	
5=Pa241	4.1238058-02	1.45377-03	-2.41552-11		5	5.0093255-02	1.28641-03	-5.20567-10	
6=Pa242	2.8833608-03	1.26819-04	-8.34691-11		6	3.3671828-03	1.22908-04	-4.87575-11	
7=Bu	-3.2372590+02	0.00000			7	2.1969518+02	0.00000		
1=U235	1.5000000+00	0.00000			1	1.4750000+00	0.00000		
2	3.6617587+00	5.23806-02	-2.40134-06	2.72228-12	2	3.5804746+00	4.66209-02	-1.85345-08	2.05738-12
3	1.1664093-01	8.18511-03	-6.00039-10		3	2.0518996-01	8.23839-03	-8.91196-10	
4	3.8866906-01	6.57825-03	-8.93687-10		4	4.2188475-01	6.22738-03	-5.85179-10	
5	5.9159596-02	1.21713-03	-1.00537-10		5	6.8424319-02	1.21822-03	-1.03002-10	
6	3.9563964-03	1.19751-04	-8.35485-11		6	4.6562419-03	1.17455-04	-1.56607-10	
7	7.6446201+02	0.00000			7	1.3107296+03	0.00000		
1	1.4500000+00	0.00000			1	1.4250000+00	0.00000		
2	3.5001076+00	4.19869-02	-1.05517-08	5.38065-13	2	3.4206633+00	3.85819-02	-7.42033-09	5-12
3	2.9374109-01	8.99439-03	-2.84370-10		3	3.8231254-01	1.00950-02	-2.30910-09	
4	4.5439645-01	6.06149-03	-2.96382-09		4	4.8619878-01	6.07083-03	-6.55905-09	
5	7.7874550-02	1.26094-03	-6.07945-10		5	8.7497291-02	1.32680-03	-1.27371-10	
6	5.4720502-03	1.16914-04	-1.39749-10		6	6.4092473-03	1.19796-04	-1.69585-11	
7	1.8586591+03	0.00000			7	2.4084181+03	0.00000		
1	1.4000000+00	0.00000			1	1.3750000+00	0.00000		

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2	1	3.3421468+00	3.64685-02	-1.64109-08	7.51513-12	2	1	3.2645639+00	3.56275-02	-1.94923-08	2	2882-12
3		4.7092363-01	1.13245-02	-1.58419-09		3		5.5959488-01	1.26004-02	-3.85010-09		
4		5.1728617-01	6.25255-03	-9.28430-09		4		5.4765293-01	6.61031-03	-7.62263-09		
5		9.7279413-02	1.41030-03	-1.35291-09		5		1.0720766-01	1.51647-03	-1.32908-09		
6		7.4733585-03	1.28270-04	-1.22518-10		6		8.6700141-03	1.44398-04	-1.91148-10		
7		2.9601809+03	0.00000			7		3.5141294+03	0.00000			
1		1.3500001+00	0.00000			1		1.3250001+00	0.00000			
2	1	3.1879202+00	3.59396-02	-7.96643-09	3.30520-12	2	1	3.1122216+00	3.72108-02	-1.73627-08	8.77145-12	
3		6.4834809-01	1.39240-02	-5.31188-09		3		7.3720648-01	1.53455-02	-1.63126-09		
4		5.7729315-01	7.15150-03	-6.54536-09		4		6.0620076-01	7.88366-03	-3.20336-09		
5		1.1726863-01	1.65694-03	-3.36053-10		5		1.2744880-01	1.84558-03	-3.09569-09		
6		1.0004954-02	1.69552-04	-2.28071-10		6		1.1484036-02	2.04362-04	-2.22361-10		
7		4.0704538+03	0.00000			7		4.6293522+03	0.00000			
1		1.3000001+00	0.00000			1		1.2750001+00	0.00000			
2	1	3.0374739+00	3.92256-02	-1.36010-08	4.51076-12	2	1	2.9636833+00	4.17925-02	-1.78703-08	4.04150-12	
3		8.2619473-01	1.69428-02	-6.34247-09		3		9.1533920-01	1.88044-02	-4.93207-09		
4		6.3436949-01	8.81199-03	-9.06487-09		4		6.6179288-01	9.93831-03	-4.56897-09		
5		1.3773445-01	2.09462-03	-1.32456-09		5		1.4811175-01	2.41220-03	-2.82873-09		
6		1.3113237-02	2.49092-04	-5.03203-11		6		1.4898666-02	3.03994-04	-3.72740-10		
7		5.1910323+03	0.00000			7		5.7557117+03	0.00000			
1		1.2500001+00	0.00000			1		1.2250001+00	0.00000			
2	1	2.8908560+00	4.47670-02	-2.32092-08	2.31419-12	2	1	2.8189985+00	4.80532-02	-8.32111-10	2.72838-12	
3		1.0046680+00	2.10167-02	-5.92796-09		3		1.0942111+00	2.36535-02	-1.00463-08		
4		6.8846423-01	1.12614-02	-1.13255-08		4		7.1437664-01	1.27779-02	-3.95631-09		
5		1.5856668-01	2.80217-03	-2.18906-09		5		1.6908506-01	3.26509-03	-3.74216-09		
6		1.6846567-02	3.69480-04	-4.09351-10		6		1.8963328-02	4.46158-04	-6.62490-10		
7		6.3236186+03	0.00000			7		6.8949929+03	0.00000			
1		1.2000001+00	0.00000			1		1.1750001+00	0.00000			
2	1	2.7481172+00	5.15967-02	-2.60277-08	3.68595-12	2	1	2.6782191+00	5.53747-02	-1.70132-08	4.98324-13	
3		1.1840007+00	2.67713-02	-8.03959-09		3		1.2740711+00	3.04088-02	-2.79055-09		
4		7.3952295-01	1.44830-02	-5.28721-09		4		7.6389574-01	1.63711-02	-7.58476-09		
5		1.7965252-01	3.79967-03	-3.74789-09		5		1.9025450-01	4.40377-03	-2.85053-09		
6		2.1255492-02	5.34817-04	-2.79956-10		6		2.3729762-02	6.36403-04	-5.60297-10		
7		7.4700870+03	0.00000			7		8.0491668+03	0.00000			
1		1.1500001+00	0.00000			1		1.1250001+00	0.00000			
2	1	2.6093109+00	5.93869-02	-1.06442-08	9.76388-13	2	1	2.5413998+00	6.36486-02	-2.13326-08	1.31018-12	
3		1.3644593+00	3.45897-02	-9.25270-09		3		1.4552048+00	3.93269-02	-9.44313-09		
4		7.8748734-01	1.84365-02	-1.05936-08		4		8.1028979-01	2.06731-02	-4.17943-09		
5		2.0087625-01	5.07500-03	-1.20370-09		5		2.1150280-01	5.81098-03	-3.80074-09		
6		2.6393016-02	7.51992-04	-5.93518-10		6		2.9252312-02	8.82780-04	-7.40638-10		
7		8.6325131+03	0.00000			7		9.2204230+03	0.00000			
1		1.1000001+00	0.00000			1		1.0750002+00	0.00000			
2	1	2.4744931+00	6.81851-02	-1.96438-08	4.71028-13							

TABLE VI (cont'd.)

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3	1.5463502+00	4.46262-02	-7.18927-11
4	8.3229478-01	2.30748-02	-1.09777-09
5	2.2211897-01	6.60949-03	-2.12976-10
6	3.2314907-02	1.03007-03	-4.00083-10
7	9.8132107+03	0.00000	
1	1.0500002+00	0.00000	

AT THE END OF PLOT NUMBER 1 THE TIME IS .9519+02 SECONDS

Z TRY OR DIE *	THEORY Y(Q(Y)=0)	I DOUBT DY	THEORY Q(Y) SHOULD BE 0	MEAN SQUARE MISS QWQ(Y)*	Z TRY OR DIE *	THEORY Y(Q(Y)=0)	I DOUBT DY	THEORY Q(Y) SHOULD BE 0	MEAN SQUARE MISS QWQ(Y)*		
2	1	3.8270580+00	6.68629-02	-1.49625-09	1.62081-12	2	1	3.7439548+00	5.91587-02	-1.51922-08	1.09630-12
3		-6.0518537-02	1.12228-02	4.16703-11		3		2.8076843-02	9.16286-03	-1.97566-10	
4		3.2014655-01	7.89337-03	-5.83263-09		4		3.5475463-01	7.12849-03	-4.97883-09	
5		4.1238058-02	1.45377-03	-2.41552-11		5		5.0093255-02	1.28641-03	-5.20567-10	
6		2.8833608-03	1.26819-04	-8.34691-11		6		3.3671828-03	1.22908-04	-4.87575-11	
7		-3.2372590+02	0.00000			7		2.1969518+02	0.00000		
1		1.5000000+00	0.00000			1		1.4750000+00	0.00000		
2	1	3.6617587+00	5.23806-02	-2.40134-08	2.72228-12	2	1	3.5804746+00	4.66209-02	-1.85345-08	2.03738-12
3		1.1664093-01	8.18511-03	-6.00039-10		3		2.0518996-01	8.23839-03	-8.91196-11	
4		3.8866906-01	6.57825-03	-8.93687-10		4		4.2188475-01	6.22738-03	-5.85179-09	
5		5.9159596-02	1.21713-03	-1.00537-10		5		6.8424319-02	1.21822-03	-1.03002-09	
6		3.9563964-03	1.19751-04	-8.35485-11		6		4.6562419-03	1.17455-04	-1.56607-10	
7		7.5446201+02	0.00000			7		1.3107296+03	0.00000		
1		1.4500000+00	0.00000			1		1.4250000+00	0.00000		
2	1	3.5001076+00	4.19869-02	-1.05517-08	5.38065-13	2	1	3.4206633+00	3.85819-02	-7.42033-09	5.77605-12
3		2.9374109-01	8.99439-03	-2.84370-10		3		3.8231254-01	1.00950-02	-2.30916-09	
4		4.5432645-01	6.06149-03	-2.96382-09		4		4.8619878-01	6.07083-03	-6.55905-09	
5		7.7874550-02	1.26094-03	-6.07945-10		5		8.7497291-02	1.32680-03	-1.27871-10	
6		5.4720502-03	1.16914-04	-1.39749-10		6		6.4092473-03	1.19796-04	-5.69585-11	
7		1.8586591+03	0.00000			7		2.4084181+03	0.00000		
1		1.4000000+00	0.00000			1		1.3750000+00	0.00000		
2	1	3.3421468+00	3.64685-02	-1.64109-08	7.51513-12	2	1	3.2645639+00	3.56275-02	-1.94923-08	2.72882-12
3		4.7092363-01	1.13245-02	-1.58419-09		3		5.5959488-01	1.26004-02	-3.85010-09	
4		5.1728617-01	6.25255-03	-9.28430-09		4		5.4765293-01	6.61031-03	-7.62263-09	
5		9.7279413-02	1.41030-03	-1.35201-09		5		1.0720766-01	1.51647-03	-1.32908-09	
6		7.4733585-03	1.28270-04	-1.22518-10		6		8.6700141-03	1.44398-04	-1.91148-10	
7		2.9601809+03	0.00000			7		3.5141294+03	0.00000		
1		1.3500001+00	0.00000			1		1.3250001+00	0.00000		
2	1	3.1872202+00	3.59396-02	-7.96643-09	3.80520-12	2	1	3.1122216+00	3.72108-02	-1.73627-08	8.77145-12
3		6.4834809-01	1.39240-02	-5.31188-09		3		7.3720648-01	1.53455-02	-1.63126-09	
4		5.7729315-01	7.15150-03	-6.54536-09		4		6.0620076-01	7.88366-03	-3.20336-09	
5		1.1726863-01	1.85694-03	-3.36053-10		5		1.2744880-01	1.84558-03	-3.09569-09	
6		1.0004954-02	1.69552-04	-2.28071-10		6		1.1484036-02	2.04362-04	-2.22361-10	

TABLE VI (Cont'd.)

7		4.0704538+03	0.00000			7		4.6293522+03	0.00000		
1		1.3000001+00	0.00000			1		1.2750001+00	0.00000		
2	1	3.0374739+00	3.92256-02	-1.36010-08	4.51076-12	2	1	2.9636833+00	4.17925-02	-1.78703-08	4.04150-12
3		8.2619473-01	1.69428-02	-6.34247-09		3		9.1533920-01	1.88044-02	-4.93207-09	
4		6.3436949-01	8.81199-03	-9.06487-09		4		6.6179288-01	9.93831-03	-4.56897-09	
5		1.3773445-01	2.69462-03	-1.32456-09		5		1.4811175-01	2.41220-03	-2.82873-09	
6		1.3113237-02	2.49092-04	-5.03203-11		6		1.4898666-02	3.03994-04	-3.72740-10	
7		5.1910323+03	0.00000			7		5.7557117+03	0.00000		
1		1.2500001+00	0.00000			1		1.2250001+00	0.00000		
2	1	2.8908500+00	4.47670-02	-2.32092-08	2.31419-12	2	1	2.8189985+00	4.80532-02	-8.32111-10	2.72838-12
3		1.0046680+00	2.10167-02	-5.92796-09		3		1.0942111+00	2.36535-02	-1.00463-08	
4		6.8846423-01	1.12614-02	-1.13255-08		4		7.1437664-01	1.27779-02	-3.95631-09	
5		1.5856668-01	2.80217-03	-2.18906-09		5		1.6908506-01	3.26509-03	-3.74216-09	
6		1.6846567-02	3.69480-04	-4.69351-10		6		1.8963328-02	4.46158-04	-6.62490-10	
7		6.3236186+03	0.00000			7		6.8949929+03	0.00000		
1		1.2000001+00	0.00000			1		1.1750001+00	0.00000		
2	1	2.7481172+00	5.15967-02	-2.60277-08	3.68595-12	2	1	2.6782191+00	5.53747-02	-1.70132-08	4.98324-13
3		1.1840007+00	2.67713-02	-3.38959-09		3		1.2740711+00	3.04088-02	-2.79055-09	
4		7.3952295-01	1.44830-02	-5.28721-09		4		7.6389574-01	1.63711-02	-7.58476-09	
5		1.7965252-01	3.79967-03	-3.74789-09		5		1.9025450-01	4.40377-03	-2.85053-09	
6		2.1255492-02	5.34817-04	-2.79956-10		6		2.3729762-02	6.36403-04	-5.60297-10	
7		7.4700870+03	0.00000			7		8.0491668+03	0.00000		
1		1.1500001+00	0.00000			1		1.1250001+00	0.00000		
2	1	2.6093109+00	5.93869-02	-1.06442-08	9.76388-13	2	1	2.5413998+00	6.36486-02	-2.13326-08	1.31018-12
3		1.3644593+00	3.45897-02	-9.25270-09		3		1.4552048+00	3.93269-02	-9.44313-09	
4		7.8748734-01	1.84365-02	-1.05936-08		4		8.1028979-01	2.06731-02	-4.17943-09	
5		2.0087625-01	5.07500-03	-1.20370-09		5		2.1150280-01	5.81098-03	-3.80074-09	
6		2.6393016-02	7.51992-04	-5.93518-10		6		2.9252312-02	8.82780-04	-7.40638-10	
7		8.6325131+03	0.00000			7		9.2204230+03	0.00000		
1		1.1000001+00	0.00000			1		1.0750002+00	0.00000		
2	1	2.4744931+00	6.81851-02	-1.96438-08	4.71028-13						
3		1.5463502+00	4.46262-02	-7.18927-11							
4		8.3229478-01	2.30748-02	-1.09777-09							
5		2.2211897-01	6.60949-03	-2.12976-10							
6		3.2314907-02	1.03007-03	-4.60083-10							
7		9.8132107+03	0.00000								
1		1.0500002+00	0.00000								

TABLE VI (Cont'd.)

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AT THE END OF PLOT NUMBER 2 THE TIME IS 1007+03SECONDS

NON-LINEAR MULTIPLE-FIELD MAXIMUM-LIKELYHOOD THEORY-MEASUREMENT CORRELATION ANALYSIS									
TAG	J	MEASUREMENT	BEST THEORY	DIFFERENCE	FITTED CURVE	DIFFERENCE	BEST THEORY	MEAN SQUARE	IS
M	I	Y(M,J) X(M,K)	YI(M,J)	DY(M,J)	YC(M,J)	(Y-YC)/SIGMA	L MISFIT Q(M,L)	MISFIT QWQ(M)	
1	Y1	1.4851000+00	1.4829240+00	2.1752475-03	1.4851000+00	0.0000000	Q1	1.3587909-02	
1	Y2	3.7910000+00	3.7701865+00	2.0813452-02	3.7774121+00	3.5812260-01	Q2	7.0474444-03	
1	Y3	0.0000000	-6.2487493-19	6.2487493-19	-7.7107915-03	7.7107916+07	Q3	6.6500454-03	
1	Y4	3.4460000-01	3.4386028-01	7.3972647-04	3.4085378-01	9.9066126-01	Q4	2.5738648-03	
1	Y5	4.7701000-02	4.7262071-02	4.3892937-04	4.6489476-02	2.2268244+00	Q5	5.5811740-04	5.5679339+00
1	Y6	3.3323000-03	3.2022692-03	1.3003075-04	3.1593161-03	2.1109731+00			GOOD
1	X1		-1.4726795-07						
2	Y1	1.4056000+00	1.4113735+00	-5.7734727-03	1.4056000+00	0.0000000	Q1	-5.7624000-02	
2	Y2	3.4604000+00	3.5365251+00	-7.6125075-02	3.5180240+00	-9.5505604-01	R2	-2.6884492-02	
2	Y3	2.4449000-01	2.5345442-01	-8.9644226-03	2.7300502-01	-3.4852310+00	Q3	-2.4734937-02	
2	Y4	4.3324000-01	4.3971085-01	-6.4708538-03	4.4717411-01	-1.8143749+00	Q4	-1.0155225-02	
2	Y5	7.0961999-02	7.3548233-02	-2.5862341-03	7.5742085-02	-3.7041573400	Q5	-8.4321086-04	1.9956970+01
2	Y6	5.0175999-03	5.0829856-03	-6.5385665-05	5.2789462-03	-2.3418652+00			BAD
2	X1		1.7357716+03						
3	Y1	1.3824000+00	1.3847628+00	-2.3628356-03	1.3824000+00	0.0000000	Q1	2.5122896-02	
3	Y2	3.4692000+00	3.4515678+00	1.7632226-02	3.4440771+00	4.2279223-01	Q2	-1.0577101-02	
3	Y3	3.4452000-01	3.4772095-01	-3.2009525-03	3.5609268-01	-1.2623073+00	Q3	-2.7846082-03	
3	Y4	4.7529000-01	4.7386662-01	1.4233844-03	4.7685867-01	-1.8995471-01	Q4	-3.3061431-04	
3	Y5	8.4475999-02	8.3718915-02	7.5708523-04	8.4631620-02	-1.0288208-01	Q5	-3.7767868-04	3.7420026+00
3	Y6	6.6017999-03	6.0278980-03	-2.6098164-05	6.1188583-03	-9.4343668-01			GOOD
3	X1		2.2454905+03						
4	Y1	1.3557000+00	1.3519766+00	3.7233973-03	1.3557000+00	0.0000000	Q1	-3.0962116-02	
4	Y2	3.3290000+00	3.3483060+00	-1.9306014-02	3.3599621+00	-5.3464872-01	Q2	2.1664502-02	
4	Y3	4.7442000-01	4.6391568-01	1.0504327-02	4.5071631-01	1.8034620+00	Q3	-2.2383615-03	
4	Y4	5.0900000-01	5.1486195-01	-5.8619536-03	5.1026095-01	-1.3995476-01	Q4	4.6172712-03	
4	Y5	9.7208999-02	9.6498752-02	7.1024694-04	9.5035640-02	1.2336490+00	Q5	2.2947355-04	1.2468813+01
4	Y6	7.2904000-03	7.3830117-03	-9.2611795-05	7.2192765-03	4.9637249-01			GOOD
4	X1		2.8341953+03						
5	Y1	1.3053000+00	1.3023505+00	3.4494842-03	1.3058000+00	0.0000000	Q1	9.8524284-04	
5	Y2	3.2066000+00	3.1950745+00	1.1525539-02	3.2056148+00	1.8485150-02	Q2	1.4084951-02	
5	Y3	6.4315999-01	6.3999882-01	3.1611761-03	6.2774929-01	1.0561724+00	Q3	1.0754313-02	
5	Y4	5.7653999-01	5.7454449-01	1.9955064-03	5.7048169-01	6.0531641-01	Q4	5.0491863-03	
5	Y5	1.1730000-01	1.1631622-01	9.8377987-04	1.1492334-01	1.1482667+00	Q5	5.9390552-04	2.1530604+00
5	Y6	9.8666999-03	9.8720347-03	-5.3348787-06	9.6826239-03	9.5927647-01			GOOD
5	X1		3.9411663+03						
6	Y1	1.2690000+00	1.2739573+00	-4.9573288-03	1.2690000+00	0.0000000	Q1	5.7606306-02	
6	Y2	3.1518000+00	3.1090646+00	4.2735346-02	3.0941937+00	1.0999099+00	Q2	-1.0347201-02	
6	Y3	7.4722999-01	7.4091280-01	6.3172004-03	7.5855113-01	-6.5651038-01	Q3	2.8060444-03	
6	Y4	6.1460999-01	6.0740527-01	7.2047271-03	6.1302925-01	1.4789519-01	Q4	1.0446372-03	

TABLE VI (Contd.)

6 Y5	1.3040000-01	1.2787376-01	2.5262364-03	1.2990829-01	2.1729783-01	Q5	-9.4899019-04	7.2053467+00	GOOD	
6 Y6	1.1567000-02	1.1545976-02	2.1023478-05	1.1861132-02	-1.3900451+00					
6 X1		4.7638948+03								
7 Y1	1.2376000+00	1.2426337+00	-5.0337398-03	1.2376000+00	0.0000000	Q1	3.0464725-03			
7 Y2	3.0038000+00	3.0156118+00	-1.1811856-02	3.0007535+00	6.1110606-02	Q2	-1.2721812-02			
7 Y3	8.5647000-01	8.5244046-01	4.0295368-03	8.7038925-01	-7.3774023-01	Q3	-3.4360909-03			
7 Y4	6.4613000-01	6.4254329-01	3.5867048-03	6.4806567-01	-1.7251242-01	Q4	-9.0101808-03			
7 Y5	1.3863000-01	1.4078158-01	-2.1515840-03	1.4287111-01	-1.7631393+00	Q5	-1.1612180-03	1.1563037+01	GOOD	
7 Y6	1.3619000-02	1.3619594-02	-5.9398472-07	1.3978910-02	-1.3655700+00					
7 X1		5.4707246+03								
8 Y1	1.1910000+00	1.1883148+00	-2.6851930-03	1.1910000+00	0.0000000	Q1	-1.6777073-02			
8 Y2	2.6481000+00	2.7371445+00	-9.0444883-03	2.8648771+00	-3.5458328-01	Q2	2.2321948-02			
8 Y3	1.0613000+00	1.0464910+00	1.4808986-02	1.0368770+00	1.0803897400	Q3	2.3406669-03			
8 Y4	6.9920000-01	7.0067611-01	-1.4761126-03	6.9788142-01	1.0889963-01	Q4	-4.1844081-04			
8 Y5	1.6215000-01	1.6347592-01	-1.3250259-03	1.6234696-01	-6.9968034-02	Q5	9.7490083-04	3.2552483+00	GOOD	
8 Y6	1.7890999-02	1.7813584-02	7.7415273-05	1.7588837-02	9.2625152-01					
8 X1		5.5289000+03								
9 Y1	1.1196000+00	1.1159437+00	3.6562919-03	1.1196000+00	0.0000000	Q1	1.3343809-02			
9 Y2	2.6766000+00	2.6531372+00	2.3462823-02	2.6632562+00	3.0035802-01	d2	-1.2307476-02			
9 Y3	1.2801000+00	1.3067713+00	-2.6671309-02	1.2935659+00	-4.9299295-01	Q3	1.4096011-02			
9 Y4	7.7700000-01	7.7254213-01	4.4578749-03	7.6905919-01	5.8788571-01	Q4	7.9284301-03			
9 Y5	1.9628000-01	1.9410102-01	2.1789774-03	1.9254807-01	1.0954958+00	Q5	2.4461260-03	4.1483355+00	GOOD	
9 Y6	2.5047000-02	2.4670354-02	3.7664541-04	2.4288844-02	1.6609715+00					
9 X1		3.1747948+03								

SUM 7.0060746+01

2.046780000000000+002	1.604132 78619039-002	BEST FIT PARAMETERS	1.557463317582160+000	1.032519890861321+000
3.777412069285501+000	1.775135095986315+000	-1.840825013963760+000	3.355597310616572-001	4.462370126833515-001
3.408537-01580671-001	2.804081794077497+000	-7.710791600350654-003	4.258499999999999+000	3.159316092360569-003
4.101999999999999-001	0.000000000000000	4.648947630128536-002	0.000000000000000	0.000000000000000

CONVERGED RUN POSITIVE DEFINATE VARIANCE-COVARIANCE MATRIX CAVEAT EMPTOR MULTIPLE SOLUTIONS
TIME=.7037+02SECONDS

The signature of a converged solution displays itself in the trends of the last five iterations. To begin with, the misfit second gradient has remained positive-definite for several iterations. This is a good indication that the iterative process is under the influence of the least squares minimum. If so, the successive application of matrix steps will quickly lead to the best fit. Both the misfit gradient and parameter changes (i.e., $DP(K)$) become increasingly reduced in size. Moreover, the predicted change in the misfit (DQQ) also becomes increasingly small and closely agrees with the actual change in misfit. The iterative process is terminated when this actual change in misfit is less than one part in 10^5 of the misfit itself, if in addition the misfit second gradient is positive-definite.

After convergence has been attained, the statistical information contained in the least squares best fit as printed out under the heading, Maximum-Likelihood Statistical Analysis. Results contained in this section of the output are not reliable unless a converged fit has been attained. First comes the best fit parameters with their one standard deviation errors (root mean square doubt). Also included are the first and second misfit gradients, etc. Notice that these numbers are not the same as for the terminal iteration but represent the improved values generated by the last iterative step. The measurement variance is the misfit divided by the number of degrees of freedom ($MM*LQ-KP=9*5-12=33$ for this problem - actually, $KP=13$ but one parameter, $P(14)$, was held constant). The measurement variance should be near unity if the fitting equations accurately describe the data and the variance-covariance matrices faithfully represent the uncertainty in the data. A value of $QQ/(MM*LQ-KP) \approx 2$, as observed in this case, is quite acceptable. The next block of output is the variance-covariance matrix $\langle DPDP \rangle$ for the fitted parameters (labeled as "mean square correlated parameter error" in the output). Finally, the error correlation matrix $\frac{DPDP}{\langle DP \rangle \langle DP \rangle}$ is printed if $LIKCON(8) \geq 2$.

The next part of the output is usually of greatest interest to the user. It consists of cross section ratios and their one standard deviation errors as derived from the fitted parameters. Again, these results are unreliable unless convergence has been attained. The alpha value shown for the fissile isotopes is calculated from the equation

$$\hat{\alpha}^i = \hat{\sigma}_c^i / \hat{\sigma}_f^i = (\hat{\sigma}_c^i / \hat{\sigma}_a^i) / (1 - \hat{\sigma}_c^i / \hat{\sigma}_a^i)$$

Next comes the graphical part of the output. First of all, the input information for the plots is recorded as part of the printed output. The data contained in the ZDZSDS cards is used to properly scale the graphs. A separate set of ZDZSDS cards are required for each plot. One card is required for each isotope. The first and third items on each card are the minimum and maximum values to be plotted for the isotope. The fourth and sixth items are the corresponding minimum and maximum positions (in inches) that determine the size of the plot. Only one isotope may have a non-zero value for the second item. This is the incremental change for the independent variable in the fitting equations which, of course, is ^{235}U in this sample case. A positive non-zero number for the fifth item indicates which isotope will be plotted on the X-axis. All other isotopes will be plotted on the Y-axis unless they have a negative number as their fifth item, in which case they will not be plotted at all. The ARTIST subroutine draws the scales and axis titles on the graphs. Graphs for this case are shown in Figures 2 and 3. They are plots of the plutonium isotopic concentrations versus burnup and ^{235}U isotopic concentration. The angular discontinuity of the lines at the beginning of the burnup graph in Figure 2 are caused by a protective feature of the plotting

Figure 2. Graphical Output for Sample Case of the Plutonium Isotopes vs. Burnup.

Figure 3. Graphical Output for Sample Case of the Plutonium Isotopes vs. ^{235}U .

subroutine which will not permit lines or points to be drawn outside of the plot boundaries. The numerical data contained in the plotted curves of the graphs is printed below the graphical input data.

The last large block of output consists of information pertinent to the individual data points. The most useful part of this information is located in the columns marked (1) Measurement (the measured values of the data point), (2) Fitted Curve (the isotopic concentration as determined by the burnup equations evaluated at the measured ^{235}U value, i.e. Y_1 , for the data point), (3) Difference $(Y-YC)/\text{SIGMA}$ (the difference between the measured and fitted isotopic values measured in standard deviations of the Y variable), (4) Mean Square Misfit (this is a measure of how far the measured data point, consisting of all isotopes, is from the fitted burnup curve), and (5) Fit Is (GOOD or BAD). A data point is labeled GOOD if the mean square misfit for the point is less than the average mean square misfit of the other data points multiplied by the input quantity labeled BAD (equal to 3.0 in the sample run). Under this criterion, all of our points are marked GOOD except the second one. The number shown for X_1 is the burnup as calculated from the fitted parameters. This value may be compared with the measured value recorded among the input data at the beginning of the printout.

The last part of the printed output consists of the double precision values of the "best fit" parameters from the final iteration and a one line summary briefly stating the status of the run. Since $\text{LIKCON}(7)=1$, the best-fit parameters are also punched out on cards. The cards obtained from the sample case are shown in Table VIII. If the case is to be rerun, these cards, can be inserted after the "P(1)=" input card in place of the original parameter guesstimates thereby saving the iteration time incurred in the preceding run.

TABLE VII

BEST FIT PARAMETERS
PUNCHED CARD OUTPUT FOR THE SAMPLE CASE

```

2.0467800000000000+002, 1.604132678619039-002, -1.840846268578366+000,
1.657413848247599+000, 1.032637957620888+000, 3.777419538762735+000,
1.775196960938419+000, -7.710973097476149-003, 8.355501241969356-001,
4.462454381260938-001, 3.408562182437419-001, 2.804075492592710+000,
4.648962794215040-002, 4.258499999999999+000, 3.159323142118266-003,
4.101999999999999-001, 0.000000000000000, 0.000000000000000,
0.000000000000000, 0.000000000000000,

```

Timing information is printed at selected places in the output. The time clock is set to zero at the start of the analysis. With this timing information the user can better estimate elapsed time requirements for other DBUFIT-I runs.

GENERAL COMMENTS

The remainder of this section contains general statements related to the use of the DBUFIT-I code. The integrated burnup equations (1-5 for plutonium systems and 6-17 for uranium-plutonium systems) were obtained under the restriction that the cross section ratios are either constant or vary as $X + XX/N^i$ over the full exposure range. This form for the cross section ratios is inadequate for describing some sets of burnup data. General experience indicates that the equations work quite well for aluminum-plutonium burnup data and also for PuO_2 enriched UO_2 burnup data. They are, however, generally inadequate for describing natural or ^{235}U enriched UO_2 fuel, although they can still be used to provide a fit to the data. Such a fit is not as good as that which could be expected if more realistic forms for the cross section ratios were employed.

The major problem of the form currently in use for ^{235}U enriched fuel is that the plutonium cross section ratios which vary inversely as their isotopic

concentration are infinite at zero burnup where the plutonium concentration is zero. Even though these cross section ratios become infinite, the burnup equations themselves are mathematically well behaved. It is mainly that they do a poor job of fitting the data because of the unreal value of the cross section ratio at low burnups. In practice, this difficulty can be partially avoided by excluding the low burnup data from the least squares fit. The resulting least squares fit and cross section ratios are more realistic. However, they are still not completely adequate because of changes that occur as a ^{235}U driven system converts itself to a plutonium driven system. These changes cause cross section ratio variations which are, in general, incompatible with the simple forms assumed to obtain the integrated burnup equations. Since ^{235}U enriched uranium is a common type of fuel, future efforts to improve the DBUFIT-I code should be primarily directed toward burnup equations employing more realistic shapes for the cross section ratios. On the other hand, the current scheme does work well for certain types of data.

A reinterpretation of those parameters concerned with the constants of integration has markedly improved the percentage of converged runs for burnup problems. The DBUFIT-I code uses the initial isotopic concentrations as parameters in place of the closely related constants of integration (the K_i of Equations 1-17) that were used in the DUBLIK code. Experience has shown that when the K_i , which are functions of the other fitting parameters, are themselves used as fitting parameters, the resulting least squares fit frequently will not properly converge but will unacceptably hang up on a least squares saddle. The reason for this is believed to be that since the K_i are functions of the other parameters, the full set of parameters are strongly correlated. The least squares code, evidently, often has difficulty in unscrambling this correlation

and therefore "hangs on a saddle". Using the initial concentrations as parameters instead of the K_i has eliminated this problem. However, the size of subroutine THEORY has been nearly doubled by this change,

In principle, every cross section ratio can be determined from the least squares fit. In practice, the burnup data is not accurate enough to determine all of them. The cross section ratio involving the absorption cross section of the Isotope described by the last equation in a group of fitted equations (e.g. $\sigma_a^{42}/\sigma_a^{25}$ in the group of Equations 11-13 or $\sigma_a^{64}/\sigma_a^{25}$ in the group 15-17) is one of these. The reason for this is most easily seen by examining the appropriate differential burnup equations. For example, consider the following consecutive equations

$$\frac{dN^{42}}{dN^{25}} = - \frac{\sigma_c^{41}}{\sigma_a^{25}} \frac{N^{41}}{N^{25}} + \frac{\sigma_a^{42}}{\sigma_a^{25}} \frac{N^{42}}{N^{25}}$$

and

$$\frac{dN^{53}}{dN^{25}} = - \frac{\sigma_a^{42}}{\sigma_a^{25}} \frac{N^{42}}{N^{25}} + \frac{\sigma_a^{53}}{\sigma_a^{25}} \frac{N^{53}}{N^{25}}$$

from the uranium-plutonium set. On the assumption that the ^{242}Pu and ^{243}Am concentrations are small to begin with and build up as the burnup progresses,

the first equation shows that the buildup term $-\frac{\sigma_c^{41}}{\sigma_a^{25}} \frac{N^{41}}{N^{25}}$ is predominant over

the burnout term $\frac{\sigma_a^{42}}{\sigma_a^{25}} \frac{N^{42}}{N^{25}}$ since $N^{41} \gg N^{42}$. This occurs as a result of the

fact that appreciable amounts of ^{241}Pu must be available before significant amounts of ^{242}Pu can be generated. Thus, a rather large discrepancy in the burnout term can be compensated for by a small adjustment in the buildup term.

Therefore, the burnup equation for ^{242}Pu serves to accurately determine

$\hat{\sigma}_c^{41}/\hat{\sigma}_a^{25}$ which occurs in the buildup term but will not permit an accurate determination of $\hat{\sigma}_a^{42}/\hat{\sigma}_a^{25}$ which occurs in the burnout term. The situation is changed, however, if experimental data is available for ^{243}Am . For in this case, $\hat{\sigma}_a^{42}/\hat{\sigma}_a^{25}$ appears in the buildup of the ^{243}Am equation and can therefore be accurately determined. This time it is $\hat{\sigma}_a^{53}/\hat{\sigma}_a^{25}$ that cannot be accurately determined. This illustrates the initial statement which says that the final absorption cross section ratio in a group of equations cannot be accurately determined from the associated burnup data and therefore must be fixed at a calculated value during the fitting process. The parameter $\sigma_c^{41}/\sigma_a^{41}$ must also be calculated and held fixed for similar reasons. Since ^{241}Pu undergoes both capture and fission, the burnup term for ^{241}Pu is not the same as the buildup term for ^{242}Pu . Thus, the cross section ratio $\hat{\sigma}_c^{41}/\hat{\sigma}_a^{25}$ term of the ^{242}Pu buildup term and the $\hat{\sigma}_a^{42}/\hat{\sigma}_a^{25}$ cross section ratio of the ^{241}Pu burnout term cannot both be accurately determined from the burnup data and one or the other must be set by the user. The $\hat{\sigma}_c^{41}/\hat{\sigma}_a^{25}$ term (which equals $(\hat{\sigma}_c^{41}/\hat{\sigma}_a^{41})(\hat{\sigma}_a^{41}/\hat{\sigma}_a^{25})$) is probably the best choice to hold fixed since $\hat{\sigma}_c^{41}/\hat{\sigma}_a^{41}$ is nearly the same for all thermal reactors. A similar situation would exist for ^{239}Pu except that experimental data on the ^{239}Pu fissions is available, so that in this instance both $\hat{\sigma}_a^{49}/\hat{\sigma}_a^{25}$ and $\hat{\sigma}_c^{49}/\hat{\sigma}_a^{25}$ can be accurately ascertained from the data.

A valid analysis of burnup data places several restrictions on the data itself. At least three data points must be available before an analysis can be undertaken. Experience suggests that good results can be obtained if the data is spaced at approximately 1000 MWd/MTM intervals of exposure. Least squares results are much better from data that is uniformly distributed than from an equivalent amount of data which is grouped in clusters.

One of the assumptions built into the burnup equations is that a single set of parameters describes all of the data. Therefore, burnup data that does not have the same initial isotopic content may not legitimately be analysed as part of the same set. Moreover, the spectral history of the samples is not to vary from sample to sample. Otherwise a unique set of cross section ratios (and hence a unique set of parameters) would not exist for all of the data points since, in general, different spectral histories (i.e., neutron spectrums) mean different flux averaged cross sections which in turn mean different cross section ratios. In practice this last requirement, which is basic to the least squares analysis of burnup data, is not always easily satisfied because economic and operational considerations are more important than the accumulation of burnup data for most reactors. However, it must be realized that data which does not fully satisfy these requirements can not be expected to yield completely reliable results. This, of course, is a matter of degree. Experience has shown that mixing data from different regions of a reactor is often a risky procedure unless one is reasonably certain that the neutron spectra and fuel temperature is the same in these regions. In cases where there is insufficient data, this requirement is usually the first to be relaxed. Clearly, cross section information obtained from this type of data should only be used with full cognizance of the problems involved.

PROPOSED IMPROVEMENTS FOR THE DBUFIT-I CODE

The DBUFIT-I code still needs several improvements. A method for removing the present restrictions on the shape of the cross section ratios deserves first priority. The problems encountered because of these restrictions are discussed in the preceding section. The removal of these restrictions is the key to the unqualified least squares analyses of burnup data from ²³⁵U enriched fuel. One

method that might work is to describe the isotopic transmutation equations in small steps of exposure using cross section ratios that are constant for each step but that are free to vary from step to step, thereby providing a reasonable approximation to any shape for the cross section ratios.

Another change that could profitably be made in the DBUFIT-I code is to have the code automatically formulate the derivatives of the burnup equations with respect to the burnup parameters instead of having to explicitly write them into subroutine THEORY as is now done. This would greatly simplify the THEORY subroutine and, incidentally, eliminate the formulation and encoding of derivatives as a potential source of error. The derivatives encoded in the current versions of the THEORY subroutines have been checked by comparing them with those obtained by a difference technique. In fact, this difference technique appears to be the best approach for forming the derivatives automatically within the least squares code.

The next version of the DBUFIT code should attempt to implement these improvements. Such a code would probably require more computation time than the present version but that should be more than offset by having a code which is more responsive to the needs of the least squares burnup problem (i.e., unrestrictive forms for the cross section ratios). An added advantage would be that the average user could easily adapt the code to his set of burnup data by encoding the appropriate burnup equations himself. This increased flexibility, that would be available to the user, occurs because he would no longer have to encode the numerous derivatives associated with the burnup equations since the code would do that for him.

ACKNOWLEDGMENT

Many fruitful discussions concerning the least squares iterative process were held with D. A. Kottwitz, The suggestions of Dr. Kottwitz are the primary source of the modifications to the Iterative **process** that have been introduced into the DBUFIT-I code.

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