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A METHOD FOR NONLINEAR EXPONENTIAL REGRESSION ANALYSIS

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16. ABSTRACT

This report presents a computer-oriented technique for performing a nonlinear exponential regression analysis on decay-type experimental data. The technique involves the least squares procedure wherein the nonlinear problem is linearized by expansion in a Taylor series. A linear curve-fit procedure for determining the initial nominal estimates for the unknown exponential model parameters is included as an integral part of this technique. A correction matrix is derived and then applied to the nominal estimate to produce an improved set of model parameters. The solution cycle is repeated until some predetermined criterion is satisfied.

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DEFINITION OF SYMBOLS

Symbol	Definition
f^o	Observed response variable
f^c	Computed response variable
t	Independent variable
A_i , B_i	Exponential regression coefficients
$\tilde{A}_i$, $\tilde{B}_i$	Initial approximations for A_i , B_i
$\bar{\Delta}$	Parameter correction matrix
V_{fi}	Residuals associated with response variable
S	Minimizing function
$\bar{W}$	Parameter weight matrix
$\bar{B}$	Partial derivative matrix
σ_o^2	Unit variance
σ_f	Standard deviation of response variable
$\tilde{F}$	Sum of squares of deviations
n	Number of data points
$(\ )\|_o$	Partial derivative evaluation at nominal estimate
m	Number of exponential terms ($n \geq 2m + 1$)

TECHNICAL MEMORANDUM X-64633

A METHOD FOR NONLINEAR EXPONENTIAL REGRESSION ANALYSIS

INTRODUCTION

The investigation of physical processes frequently requires the use of models that simulate or describe the processes. A model is often chosen so that certain variables interact in the model according to physical theories associated with the particular process. Formulation of a model often results in the form referred to as mathematical models. This is the familiar representation of the physical process by one or more equations that encompass the physical theory. A model equation contains identified independent variables and unknown parameters. Regression analysis is the statistical tool used to determine these unknown parameters, thereby providing an analytical representation of the experimental data.

The general procedure in regression analysis is to take partial derivatives of a specific model-dependent minimizing function. These partial derivatives are taken with respect to each of the unknown model parameters. If the set of equations obtained by setting these partial derivatives equal to zero can be solved by the usual algebraic methods, the fitting or analytical representation is accomplished. However, if these equations are transcendental in one or more of the unknown parameters, they cannot be solved by the usual algebraic methods.

The processes of particular interest in this report are those that can be described by decaying exponential forms. A mathematical model that contains more than one exponential term results in a set of transcendental normal equations if conventional forms of regression analysis are used. Thus, one usually resorts to iterative methods that require initial estimates for the parameters. The method described herein involves the least squares procedure, whereby the nonlinear problem is linearized by expanding in a Taylor series. In this iterative method, we first develop a starting nominal guess for the model parameters. A correction matrix is derived and then applied to the nominal guess to produce an improved set of model parameters. This procedure is continued until some predetermined criterion is satisfied. The number of iterations necessary for convergence is closely related to this criterion, the initial estimates, and the form of the exponential model.

Additional information on the various methods of curve-fitting decay-type data to a sum of exponentials is given in References 1 through 5. Procedures for obtaining the initial parameter estimates are discussed in References 6 through 8. It is noted that the initial estimate procedure herein is not restricted to equally spaced data.

Application of the procedure is illustrated with data obtained from a particular process concerning the anodic oxidation of metals. In this process one expects an exponential or logarithmic behavior. From an analysis of the results, it is concluded that an adequate two-term exponential representation of the data is obtained. Thus, the analytical representation of the physical process data is accomplished using an exponential decay-type model.

MATHEMATICAL THEORY FOR EXPONENTIAL REGRESSION ANALYSIS

In general, we are given the set of observed values $\{(t_1, f_1^o), (t_2, f_2^o), \ldots, (t_n, f_n^o)\}$. We assume that the function to be fitted to these data is of the following form:

$$f^c = A_1 e^{-B_1 t} + A_2 e^{-B_2 t} + \ldots + A_m e^{-B_m t} + K \equiv f(A, B, K, t) \quad , \qquad (1)$$

where f^c represents the calculated value of the response and K, A_i, $B_i (i = 1, 2, \ldots, m)$ are the $2m + 1$ parameters to be estimated. The independent variable is time t. We first consider the simple case $m = 1$ and $K = 0$ which results in a conventional least squares solution for the unknowns A_1 and B_1. We have the following model:

$$f^c = A_1 e^{-B_1 t} \quad . \qquad (2)$$

By taking the natural log of both sides,

$$\ln f^c = \ln A_1 - B_1 t \quad . \qquad (3)$$

Let

$$\left.\begin{aligned} C &= \ln A_1 \\ &\text{and} \\ Y &= \ln f^{o} \end{aligned}\right\} \quad . \tag{4}$$

Then,

$$Y = C - B_1 t \quad . \tag{5}$$

The least squares solutions for C and B_1 then become

$$B_1 = -\left[\frac{m \sum_{i=1}^{n} t_i Y_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} Y_i}{m \sum_{i=1}^{n} t_i^2 - \left(\sum_{i=1}^{n} t_i\right)^2}\right] \tag{6}$$

and

$$C = \left[\frac{\sum_{i=1}^{n} t_i^2 \sum_{i=1}^{n} Y_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} t_i Y_i}{m \sum_{i=1}^{n} t_i^2 - \left(\sum_{i=1}^{n} t_i\right)^2}\right] \quad . \tag{7}$$

For $m > 1$ and $K \neq 0$ we proceed as follows. We write the parameters as initial approximations or nominal values plus unknown corrections; that is,

$$\left.\begin{aligned}
A_1 &= \tilde{A}_1 + \Delta A_1 \\
B_1 &= \tilde{B}_1 + \Delta B_1 \\
A_2 &= \tilde{A}_2 + \Delta A_2 \\
B_2 &= \tilde{B}_2 + \Delta B_2 \\
&\;\;\vdots \\
A_m &= \tilde{A}_m + \Delta A_m \\
B_m &= \tilde{B}_m + \Delta B_m \\
K &= \tilde{K} + \Delta K
\end{aligned}\right\} \quad . \tag{8}$$

For any assumed functional form, the following condition equation can be written:

$$f_i^o - f_i^c - V_{fi} = 0 \quad , \tag{9}$$

where

f_i^o = observed values of the response variable,

f_i^c = calculated values of the response variable,

and

V_{fi} = residuals associated with the response variable.

If we substitute equation (8) into equation (1) and the result into equation (9), we obtain

$$f_i^o - f_i\Big(\tilde{A}_1 + \Delta A_1\,,\ \tilde{B}_1 + \Delta B_1\,,\ \ldots\,,\ \tilde{A}_m + \Delta A_m\,,\ \tilde{B}_m + \Delta B_m\,,$$

$$\tilde{K} + \Delta K,\ t\Big) - V_{fi} = 0 \quad , \tag{10}$$

or

$$f_i\left(\tilde{A}_1 + \Delta A_1 , \tilde{B}_1 + \Delta B_1 , \ldots , \tilde{A}_m + \Delta A_m , \tilde{B}_m + \Delta B_m ,\right.$$

$$\left.\tilde{K} + \Delta K, t\right) = f_i^o - V_{fi} \quad . \tag{11}$$

Expanding the left side of equation (11) in a Taylor series about the estimates $\tilde{A}_1 , \tilde{B}_1 , \ldots , \tilde{A}_m , \tilde{B}_m , \tilde{K}$ and neglecting higher order terms than the first, we have $(i = 1, 2, \ldots , n)$

$$V_{fi} = N_i - F_{1i}\,\Delta A_1 - F_{2i}\,\Delta B_1 - F_{3i}\,\Delta A_2 - F_{4i}\,\Delta B_2 - \ldots$$

$$- F_{2m-1,i}\,\Delta A_m - F_{2m,i}\,\Delta B_m - F_{2m+1,i}\,\Delta K \quad , \tag{12}$$

where

$$\left.\begin{aligned}
F_{1i} &= \left.\frac{\partial f_i}{\partial A_1}\right|_o & F_{4i} &= \left.\frac{\partial f_i}{\partial B_2}\right|_o \\
& & &\vdots \\
F_{2i} &= \left.\frac{\partial f_i}{\partial B_1}\right|_o & F_{2m-1,i} &= \left.\frac{\partial f_i}{\partial A_m}\right|_o \\
F_{3i} &= \left.\frac{\partial f_i}{\partial A_2}\right|_o & F_{2m,i} &= \left.\frac{\partial f_i}{\partial B_m}\right|_o \\
& & F_{2m+1,i} &= \left.\frac{\partial f_i}{\partial K}\right|_o
\end{aligned}\right\} \tag{13}$$

and

$$N_i = f_i^o - f_i\,(\tilde{A},\ \tilde{B},\ \tilde{K},\ t) \qquad . \tag{14}$$

The n equations given by equation (12) are the linearized condition or residual equations. According to the Gauss least squares principle, the best representation of the data is that which makes the weighted sum of the squares of the residuals a minimum. Thus, the minimizing function is

$$\begin{aligned} S &= f\left(\Delta A_1\,,\ \Delta B_1\,,\ \ldots\,,\ \Delta A_m\,,\ \Delta B_m\,,\ \Delta K\right) \\ &= W_1 V_{f1}^2 + W_2 V_{f2}^2 + \ldots + W_n V_{fn}^2 \qquad . \end{aligned} \tag{15}$$

The $2m + 1$ linear algebraic equations for determining the Δ increments to the initial estimates are now obtained by taking the partial derivative of S with respect to each of the unknown corrections and setting the result equal to zero. These equations, frequently referred to as the normal equations, are given by

$$\left.\begin{aligned} \frac{\partial S}{\partial \Delta A_1} &= 2W_1 V_{f1} \frac{\partial V_{f1}}{\partial \Delta A_1} + 2W_2 V_{f2} \frac{\partial V_{f2}}{\partial \Delta A_1} + \ldots + 2W_n \frac{\partial V_{fn}}{\partial \Delta A_1} = 0 \\ \frac{\partial S}{\partial \Delta B_1} &= 2W_1 V_{f1} \frac{\partial V_{f1}}{\partial \Delta B_1} + 2W_2 V_{f2} \frac{\partial V_{f2}}{\partial \Delta B_1} + \ldots + 2W_n \frac{\partial V_{fn}}{\partial \Delta B_1} = 0 \\ &\ \ \vdots \\ \frac{\partial S}{\partial \Delta K} &= 2W_1 V_{f1} \frac{\partial V_{f1}}{\partial \Delta K} + 2W_2 V_{f2} \frac{\partial V_{f2}}{\partial \Delta K} + \ldots + 2W_n \frac{\partial V_{fn}}{\partial \Delta K} = 0 \end{aligned}\right\} \tag{16}$$

or

$$\left.\begin{aligned}
& -W_1V_{f1}F_{11} - W_2V_{f2}F_{12} - \cdots - W_nV_{fn}F_{1n} = 0 \\
& -W_1V_{f1}F_{21} - W_2V_{f2}F_{22} - \cdots - W_nV_{fn}F_{2n} = 0 \\
& \qquad\qquad\qquad\qquad\qquad \vdots \\
& -W_1V_{f1}F_{2m+1,1} - W_2V_{f2}F_{2m+1,1} - \cdots - W_nV_{fn}F_{2m+1,n} = 0
\end{aligned}\right\} \quad . \tag{17}$$

We now express equation (12) in the following more convenient matrix expression

$$\overline{V} + \overline{B}\,\overline{\Delta} - \overline{N} = 0 \quad , \tag{18}$$

where

$$\underset{[n\times 1]}{\overline{V}} = \begin{bmatrix} V_{f1} \\ V_{f2} \\ \vdots \\ V_{fn} \end{bmatrix} \quad , \tag{19}$$

$$\underset{[n\times(2m+1)]}{\overline{B}} = \begin{bmatrix} F_{11} & F_{21} & \cdots & F_{2m+1,1} \\ F_{12} & F_{22} & \cdots & F_{2m+1,2} \\ \vdots & \vdots & & \vdots \\ F_{1n} & F_{2n} & \cdots & F_{2m+1,n} \end{bmatrix} \quad , \tag{20}$$

$$\underset{[(2m+1)\times 1]}{\overline{\Delta}} = \begin{bmatrix} \Delta A_1 \\ \Delta B_1 \\ \Delta A_2 \\ \Delta B_2 \\ \vdots \\ \Delta A_m \\ \Delta B_m \\ \Delta K \end{bmatrix} \quad , \tag{21}$$

and

$$\underset{[n\times 1]}{\overline{N}} = \begin{bmatrix} N_1 \\ N_2 \\ \vdots \\ N_n \end{bmatrix} \quad . \tag{22}$$

By using the denotations for $\overline{V}$ and $\overline{B}$ as given by equations (19) and (20), respectively, we can also rewrite equation (17) as

$$\overline{B}^T \, \overline{W} \, \overline{V} = 0 \quad , \tag{23}$$

where

$$\underset{[n\times n]}{\overline{W}} = \begin{bmatrix} \sigma_o^2/\sigma_{f1}^2 & 0 & \dots & 0 \\ 0 & \sigma_o^2/\sigma_{f2}^2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \sigma_o^2/\sigma_{fn}^2 \end{bmatrix} \quad . \tag{24}$$

Solving equation (18) for $\overline{V}$,

$$\overline{V} = \overline{N} - \overline{B}\,\overline{\Delta} \quad . \tag{25}$$

Substituting equation (25) into equation (23),

$$\overline{B}^T \overline{W} (\overline{N} - \overline{B}\,\overline{\Delta}) = 0 \quad . \tag{26}$$

Solving for $\overline{\Delta}$,

$$\overline{B}^T \overline{W}\,\overline{N} - \overline{B}^T \overline{W}\,\overline{B}\,\overline{\Delta} = 0 \tag{27}$$

or

$$\overline{\Delta} = (\overline{B}^T \overline{W}\,\overline{B})^{-1} (\overline{B}^T \overline{W}\,\overline{N}) \quad . \tag{28}$$

An improved set of values for the parameters is then given by equation (8). The process or cycle is repeated to produce the corrections resulting from the second cycle. These corrections are then added to the estimates from the first cycle:

$$\left.\begin{aligned} A_1^1 &= \Delta A_1^1 + A_1 \\ B_1^1 &= \Delta B_1^1 + B_1 \\ A_2^1 &= \Delta A_2^1 + A_2 \\ B_2^1 &= \Delta B_2^1 + B_2 \\ &\vdots \\ A_m^1 &= \Delta A_m^1 + A_m \\ B_m^1 &= \Delta B_m^1 + B_m \\ K^1 &= \Delta K^1 + K \end{aligned}\right\} \quad . \tag{29}$$

These values represent an improved set of estimates to use for the third cycle. An iterative procedure is thus set up for improving the parameter estimates to any prescribed degree of accuracy consistent with the accuracy of the observed data.

The standard algorithm is based on obtaining a nominal solution that, hopefully, converges to the correct solution. The algorithm is summarized as follows:

1. Let $\tilde{A}^k$ denote the kth nominal; linearize about $\tilde{A}^k$.

2. Solve the resulting linear least squares problem.

3. Use the new solution as the new nominal.

4. Check for convergence. If convergence has not occurred, repeat steps 1 through 3.

The standard deviation of each of the converged parameters is calculated from

$$\bar{\sigma} = \sigma_f \, \bar{c} \quad , \tag{30}$$

where

$$\sigma_f = \left[\frac{\sum_{i=1}^{n} \left(f_i^o - f_i^c \right)^2}{n - 2m - 1} \right]^{1/2} \tag{31}$$

and

$$\underset{[(2m+1)\times 1]}{\bar{c}} = \begin{bmatrix} \sqrt{c_{11}} \\ \sqrt{c_{22}} \\ \vdots \\ \sqrt{c_{2m+1,\,2m+1}} \end{bmatrix} \quad . \tag{32}$$

The c elements in equation (32) refer to diagonal elements in the inverse matrix $(\overline{B}^T \overline{W} \overline{B})^{-1}$.

PROCEDURE FOR OBTAINING THE INITIAL PARAMETER ESTIMATES

"Peeling-Off" Approach

An iterative method for nonlinear exponential regression analysis was developed in the previous section. Inherent in this method is a requirement for initial estimates of the parameters. This section presents a least squares "peeling-off" procedure for arriving at these initial estimates.

Our assumed exponential model is of the form given by equation (1). Generally speaking, if we plot decay-type data in the form $\ln f^o$ against t where f^o is the observed response and t is the independent variable, then for large t the curve is approximately a straight line. Consider the following Figure 1.

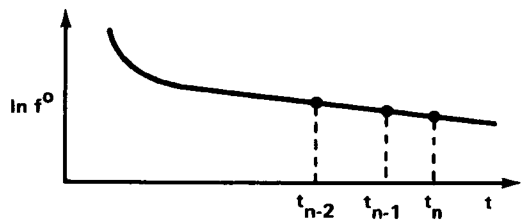

Figure 1. Logarithmic time decay illustration.

If we fit a straight line to the last three data points by the method of least squares, the assumed form is

$$\ln f^o = -\tilde{B}_m t + D \quad . \tag{33}$$

However, this is equivalent to the equation

$$f^o = \tilde{A}_m e^{-\tilde{B}_m t} \quad ,$$

where

$$D = \ln \tilde{A}_m \quad . \tag{34}$$

The coefficients $\tilde{B}_m$ and D are given by

$$D = \frac{\sum_{i=n}^{n-2} t_i^2 \sum_{i=n}^{n-2} \ln f_i^o - \sum_{i=n}^{n-2} t_i \sum_{i=n}^{n-2} t_i \ln f_i^o}{3 \sum_{i=n}^{n-2} t_i^2 - \left(\sum_{i=n}^{n-2} t_i \right)^2} \tag{35}$$

and

$$\tilde{B}_m = - \left[\frac{3 \sum_{i=n}^{n-2} t_i \ln f_i^o - \sum_{i=n}^{n-2} t_i \sum_{i=n}^{n-2} \ln f_i^o}{3 \sum_{i=n}^{n-2} t_i^2 - \left(\sum_{i=n}^{n-2} t_i \right)^2} \right] \quad . \tag{36}$$

Thus, we have determined the least squares values for $\tilde{A}_m$ and $\tilde{B}_m$. We can then obtain values for the residuals from $(i = 0, 1, 2)$

$$R_{n-i} = f_{n-i}^o - \tilde{A}_m e^{-\tilde{B}_m t_{n-i}} \quad . \tag{37}$$

We now take the next three data points at t_{n-3}, t_{n-4}, and t_{n-5} and subtract the corresponding term $\tilde{A}_m e^{-\tilde{B}_m t}$ and the arbitrary constant $\tilde{K}$ from f^o to obtain the following residuals

$$\left.\begin{aligned}
R_{n-3} &= f^{o}_{n-3} - \tilde{A}_m e^{-\tilde{B}_m t_{n-3}} - \tilde{K} \\
R_{n-4} &= f^{o}_{n-4} - \tilde{A}_m e^{-\tilde{B}_m t_{n-4}} - \tilde{K} \\
R_{n-5} &= f^{o}_{n-5} - \tilde{A}_m e^{-\tilde{B}_m t_{n-5}} - \tilde{K}
\end{aligned}\right\} . \tag{38}$$

Next, a straight line is fitted to the data for $\ln|R_{n-i}|$ against t_{n-i}, $i = 3,4,5$. This determines $\tilde{A}_{m-1}$ and $\tilde{B}_{m-1}$. The residuals for the next three data points are determined from

$$\left.\begin{aligned}
R_{n-6} &= f^{o}_{n-6} - \tilde{A}_{m-1} e^{-\tilde{B}_{m-1} t_{n-6}} - \tilde{A}_m e^{-\tilde{B}_m t_{n-6}} - \tilde{K} \\
R_{n-7} &= f^{o}_{n-7} - \tilde{A}_{m-1} e^{-\tilde{B}_{m-1} t_{n-7}} - \tilde{A}_m e^{-\tilde{B}_m t_{n-7}} - \tilde{K} \\
R_{n-8} &= f^{o}_{n-8} - \tilde{A}_{m-1} e^{-\tilde{B}_{m-1} t_{n-8}} - \tilde{A}_m e^{-\tilde{B}_m t_{n-8}} - \tilde{K}
\end{aligned}\right\} . \tag{39}$$

We now fit a straight line to $\ln|R_{n-i}|$ against t_{n-i}, $i = 6,7,8$. This determines $\tilde{A}_{m-2}$ and $\tilde{B}_{m-2}$. We continue this process until all the $\tilde{A}$'s and $\tilde{B}$'s are determined. In general, $\tilde{A}_1$ and $\tilde{B}_1$ are determined from a set that contains more than three data points. That is, the points remaining after $\tilde{A}_2$ and $\tilde{B}_2$ have been determined are used for determining $\tilde{A}_1$ and $\tilde{B}_1$. It is noted that since three points are chosen as a minimum for calculating a particular $\tilde{A}$ and $\tilde{B}$, we must have $n \geq 3m$ where n is the number of data points. At this point we calculate the weighted sum of squares of the deviations using the initial parameter estimates

$$\tilde{F}_1 = \sum_{i=1}^{n} W_i \left(f_i^o - f_i^c\right)^2 \quad , \tag{40}$$

where

$$W_i = 1/\sigma_{fi}^2 \quad ,$$

$$f_i^o = \text{observed response} \quad ,$$

and

$$f_i^c = \text{fitted response.}$$

Iteration Philosophy

The iteration logic can be summarized by the following steps:

1. Repeat the process, but use the last four data points to obtain the initial estimates of $\tilde{A}_m$ and $\tilde{B}_m$. The next three data points are used to obtain $\tilde{A}_{m-1}$, $\tilde{B}_{m-1}$, etc., for other $\tilde{A}$'s and $\tilde{B}$'s. This yields a second set of parameter estimates from which we can calculate another $\tilde{F}$; call it $\tilde{F}_2$.

2. Use the last five data points and obtain a third set of parameters which yield $\tilde{F}_3$.

3. We continue this, always keeping three points as a minimum in determining $\tilde{A}_i$ and $\tilde{B}_i$.

4. Increase the constant to $\tilde{K} + 0.05\,\tilde{K}$ and repeat steps 1 through 3. Terminate when the constant reaches a predetermined value.

5. Parameter estimates yielding the minimum $\tilde{F}$ are chosen as the initial estimates.

COMPUTER PROGRAM DEVELOPMENT

The computer programs to implement the previously developed theory for exponential regression analysis were organized and developed according to two general types of exponential models. One concerns a single exponential and the sum of exponentials without a constant, and the other concerns the sum of exponentials with a constant included. Two highly flexible computer programs were thus developed for the MSFC UNIVAC 1108 digital computer. Each program contains double-precision capability and SC-4020 plotting procedures. In addition, the "peeling-off" procedure for obtaining initial parameter estimates is an integral part of each program segment.

The logic flow for Programs I and II is depicted in Figures 2 and 3. The parameter NCASES is the number of cases of data processed in each program. The models that can be investigated in Program I are

Model I: $$f^c = A_1 e^{-B_1 t} + A_2 e^{-B_2 t} + A_3 e^{-B_3 t} + K$$

and

Model II: $$f^c = A_1 e^{-B_1 t} + A_2 e^{-B_2 t} + K \quad .$$

Those models that can be investigated in Program II are

Model III: $$f^c = A_1 e^{-B_1 t} + A_2 e^{-B_2 t} + A_3 e^{-B_3 t} \quad ,$$

Model IV: $$f^c = A_1 e^{-B_1 t} + A_2 e^{-B_2 t} \quad ,$$

and

Model V: $$f^c = A_1 e^{-B_1 t} \quad .$$

The characteristics of both programs are summarized in Table 1. It should be noted that both programs can be easily extended to include additional exponential terms if desired.

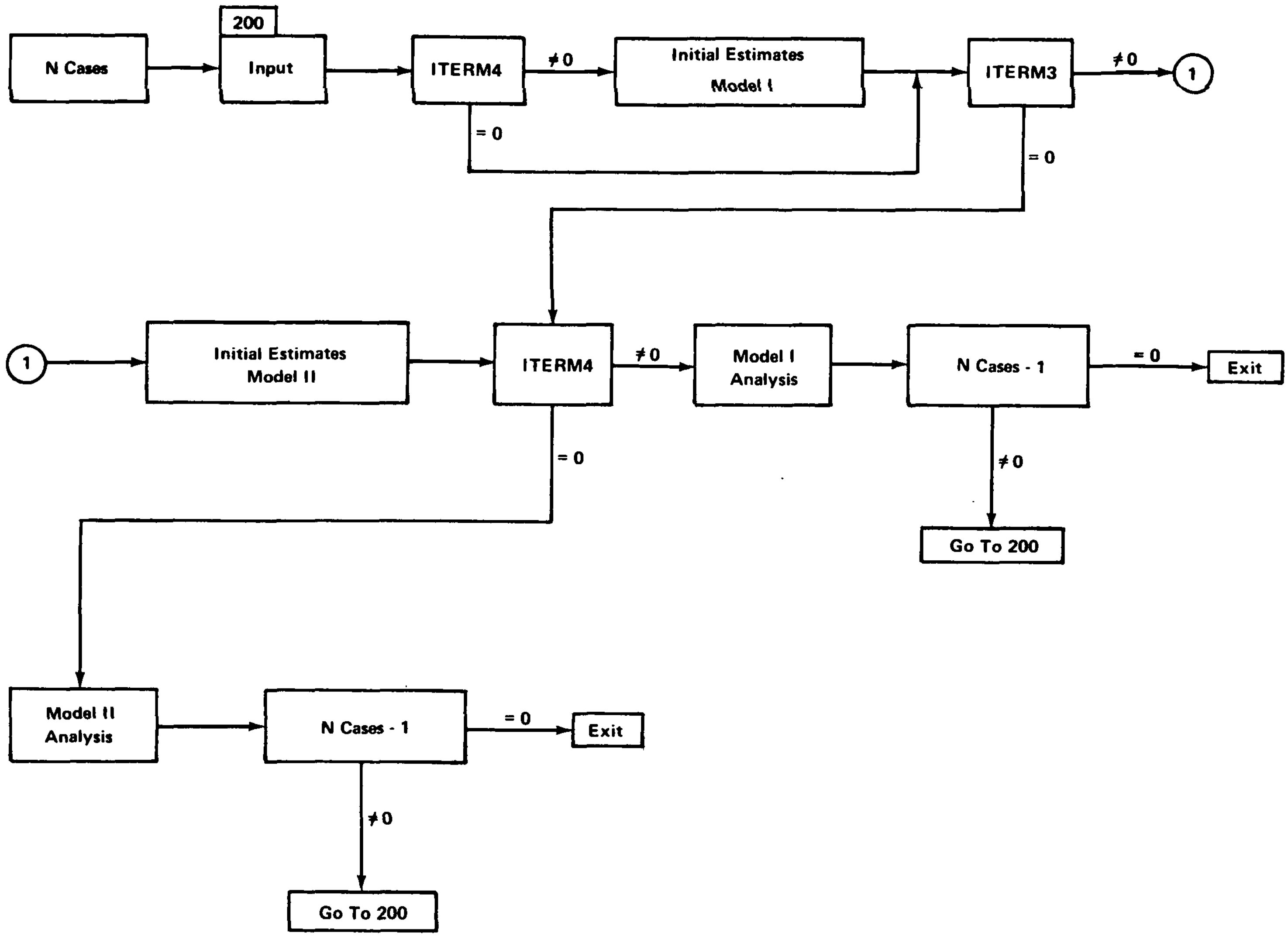

Figure 2. Program I block diagram summary.

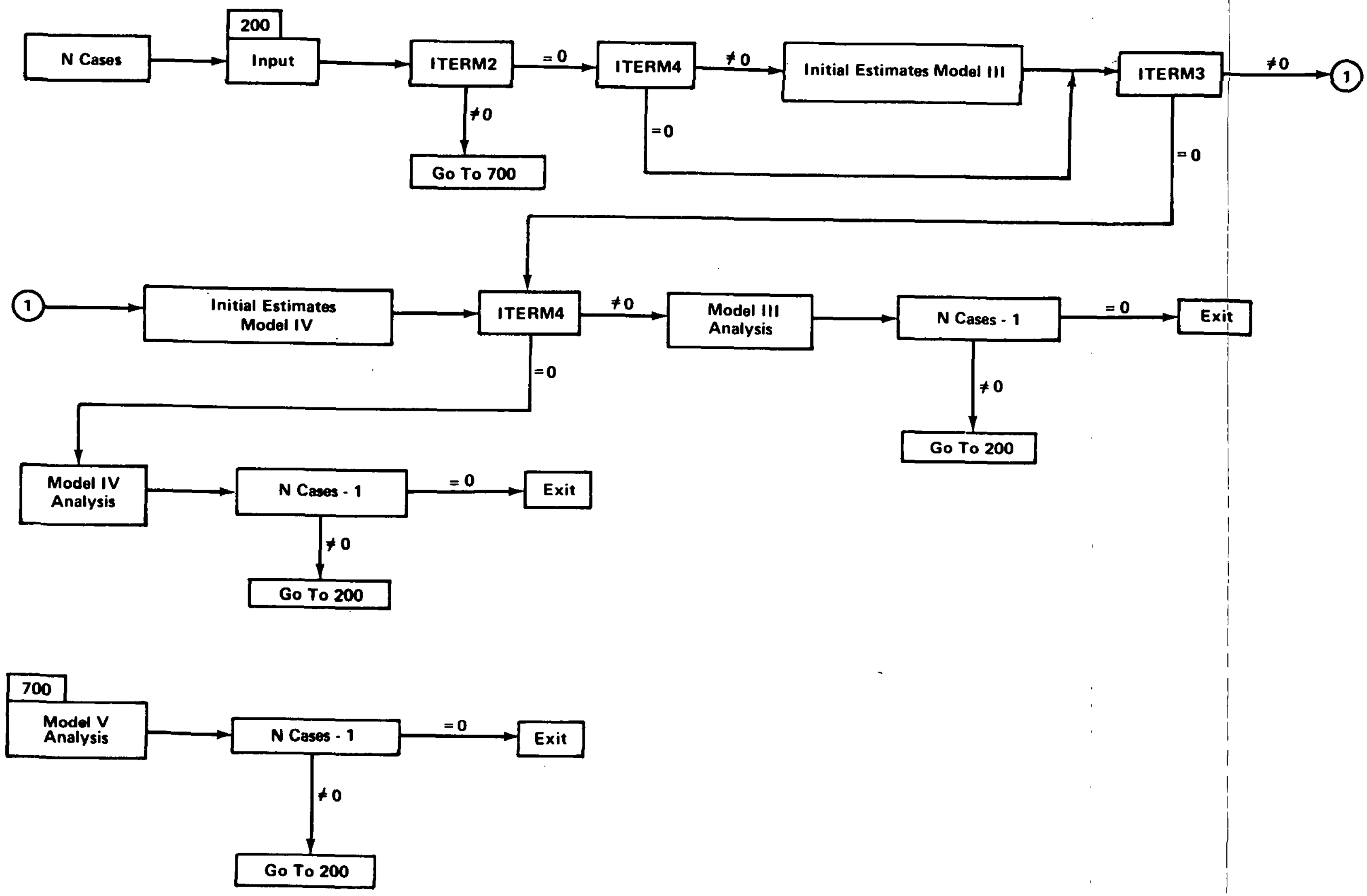

Figure 3. Program II block diagram summary.

TABLE 1. COMPUTER PROGRAM SUMMARY FOR EXPONENTIAL CURVE FITTING

Program Number[a]	Exponential Model Fitted
I	(1) A_i, B_i, $K : i = 1, 2, 3$
	(2) A_i, B_i, $K : i = 1, 2$
II	(1) A_i, $B_i : i = 1, 2, 3$
	(2) A_i, $B_i : i = 1, 2$
	(3) A_1, B_1

a. Each program has a built-in capability for obtaining initial parameter estimates.

The parameter ITERM is used to determine control transfer in each program. For example, if ITERM has the value one, parameters for the particular model associated with it are determined. A value of zero indicates that parameters for the associated model are not determined. A double-precision matrix inverse routine using the Gaussian elimination procedure is used in each program.

RESULTS AND CONCLUSIONS

Discussion of the Physical Process

In an open circuit transient analysis of the anodic oxidation of metals, one expects an exponential or logarithmic behavior. This fact is evident from the experimental data when the layer is passive; that is, normal growth is taking place. In some cases, however, growth is truncated by the onset of oxygen evolution. In this region we have electronic conduction in addition to a small amount of anodic or growth conduction. During the open circuit break, therefore, we expect the conduction to be initially dominated by electrons and as the voltage decreases, the conduction becomes primarily anodic conduction. Thus, the transient analysis has to have the capability to consider two or more conduction mechanisms, each with different relaxation times.

Basically, the voltage data from the anodic oxidation process are classified into four sets. Each set of data represents a different time held in oxygen evolution. When plotted as a function of time, these voltage data exhibit an exponential or decay-type behavior. The response data are represented as an observed voltage, which is designated as f^o.

Discussion of Results

The observed decay data were processed through both Programs I and II to assess the validity of the various exponential models. A summary of the initial estimates for the various assumed models is presented in Tables 2, 3, and 4. The minimum value for the $\tilde{F}$ quantity associated with the selected initial estimates is given in these tables.

TABLE 2. INITIAL ESTIMATE SUMMARY FOR TWO-TERM EXPONENTIAL MODEL PLUS A CONSTANT

	Set 1	Set 2	Set 3	Set 4
Groups of Initial Estimates	441	441	441	441
Group Number with Smallest $\tilde{F}$	49	44	61	63
Smallest $\tilde{F}$ Value	0.2083	0.3113	2.9021	5.986

TABLE 3. INITIAL ESTIMATE SUMMARY FOR TWO-TERM EXPONENTIAL MODEL

	Set 1	Set 2	Set 3	Set 4
Groups of Initial Estimates	63	63	63	63
Group Number with Smallest $\tilde{F}$	52	63	61	59
Smallest $\tilde{F}$ Value	0.0827	0.0455	0.01185	0.02952

TABLE 4. INITIAL ESTIMATE SUMMARY FOR THREE-TERM EXPONENTIAL MODEL PLUS A CONSTANT

	Set 1	Set 2	Set 3	Set 4
Groups of Initial Estimates	420	420	420	—
Group Number with Smallest $\tilde{F}$	59	47	14	—
Smallest $\tilde{F}$ Value	0.2132	0.3532	57.45	—

Numerical problems were encountered for both the three-term model and the three-term plus a constant model. As indicated in Table 5, divergence occurred for the set 2 and set 3 data. It is noted that the determinant of the coefficients for solving for the correction matrix was 0.911×10^{-18} in one case and 0.162×10^{-2} in the other case. Convergence failed to occur for the set 2 data even with relatively good initial estimates.

TABLE 5. RESULTS FOR THREE-TERM EXPONENTIAL MODEL PLUS A CONSTANT

Data Set Number	Set 1		Set 2		Set 3		Set 4[b]	
Parameter and Error Estimate	Initial Estimate	Improved Estimate	Initial Estimate	Improved Estimate[a]	Initial Estimate	Improved Estimate[a]	Initial Estimate	Improved Estimate
A_1	0.506027	0.550958	0.524024		0.289545			
σ	—	0.0319	—		—			
B_1	1.144510	1.003510	0.121633		0.006907			
σ	—	0.3064	—		—			
A_2	0.525248	0.571808	0.036133		0.237985			
σ	—	0.0200	—		—			
B_2	0.117757	0.063911	0.065537		0.000905			
σ	—	0.0070	—		—			
A_3	0.231458	0.108318	0.473872		0.777985			
σ	—	0.0066	—		—			
B_3	0.010038	0.012974	0.011831		0.006935			
σ	—	0.0005	—		—			
K	0.0525	0.0689	0.0770		0.21350			
σ	—	0.0039	—		—			
σ_f	0.0591	0.0321	0.0761	—	0.9705			
Determinant Value	—	7.90	—	0.0016	—	0.911×10^{-18}		

a. Diverged.

b. Numerical problems for assumed model.

The data in Table 6 summarize the results for the two-term plus a constant model. As shown in this table convergence failed to occur for the set 3 and set 4 data. The initial estimates for the set 1 and set 2 data showed some disagreement with the cycle 1 estimates. The σ_f initial estimate values for set 1 and set 2 are significantly smaller than the σ_f values at the end of cycle 1. Rather high error estimates for the A_1 and B_1 parameters are also evident in this table.

Results obtained for the two-term exponential model are perhaps the most encouraging from the standpoint of adequately describing the data. As indicated in Table 7, highly accurate parameter estimates were obtained. The converged estimates represent an improvement over the initial estimates with the exception of the set 4 data. Here it is noted that $\sigma_f = 0.0215$ for the initial estimates as compared to $\sigma_f = 0.0600$ for the improved estimates. The initial estimates were thus chosen as the representation for the set 4 data. The models that appear to adequately describe the observation data are

$$\text{Set 1:}\ f^c = 0.924798e^{-0.160783t} + 0.230238e^{-0.010751t} ,$$

$$\text{Set 2:}\ f^c = 0.629470e^{-0.23023t} + 0.676240e^{-0.01642t} ,$$

$$\text{Set 3:}\ f^c = 0.598702e^{-0.126326t} + 0.707297e^{-0.006132t} ,$$

and

$$\text{Set 4:}\ f^c = 0.424970e^{-0.109368t} + 0.897037e^{-0.005876t} .$$

The observation data and the models evaluated at the corresponding time point are presented in graphical form in Figures 4 through 7. Residual data are presented in Figures 8 through 11. These figures indicate an adequate model representation of the data. It is concluded that changing the exponential functional form for these data to one other than a two-term model is not warranted in view of the problems encountered with the other models.

The coefficients for each model are plotted in Figure 12 as a function of the time to oxygen evolution associated with each set. These data enable one to simulate the physical process using a two-term exponential model at conditions other than those tested.

TABLE 6. RESULTS FOR TWO-TERM EXPONENTIAL MODEL PLUS A CONSTANT

Data Set Number	Set 1		Set 2		Set 3		Set 4	
Parameter and Error Estimate	Initial Estimate	Cycle 1 Estimate	Initial Estimate	Cycle 1 Estimate	Initial Estimate	Cycle 1 Estimate[a]	Initial Estimate	Cycle 1 Estimate[a]
A_1	0.912635	0.826217	0.673531	0.315643	0.332689		0.023109	
σ	—	0.4746	—	0.2146	—		—	
B_1	0.158482	0.206468	0.113233	0.218638	0.287924		0.065336	
σ	—	0.1355	—	0.0569	—		—	
A_2	0.169134	0.472633	0.437571	0.414676	0.746388		0.948405	
σ	—	0.1237	—	0.0759	—		—	
B_2	0.006810	0.067656	0.011059	0.049739	0.006686		0.006476	
σ	—	0.0123	—	0.0035	—		—	
K	0.05250	0.834446	0.0770	0.55022	0.21350		0.29750	
σ	—	0.0840	—	0.0431	—		—	
σ_f	0.0575	0.6926	0.0703	0.3556	0.21463	—	0.3059	—
Determinant Value	—	$0.9687 \cdot 10^4$	—	$0.7801 \cdot 10^5$	—	$0.8811 \cdot 10^4$	—	129.94

a. Diverged.

TABLE 7. RESULTS FOR TWO-TERM EXPONENTIAL MODEL

Data Set Number	Set 1		Set 2		Set 3		Set 4	
Parameter and Error Estimate	Initial Estimate	Improved Estimate	Initial Estimate	Improved Estimate	Initial Estimate	Improved Estimate	Initial Estimate	Improved Estimate
A_1	0.951721	0.924798	0.696720	0.629470	0.593509	0.598702	0.424970	0.488538
σ	—	0.0224	—	0.0161	—	0.0065	—	0.0357
B_1	0.140500	0.160783	0.256310	0.230230	0.182970	0.126326	0.109368	0.036581
σ	—	0.0054	—	0.0109	—	0.0033	—	0.0144
A_2	0.181307	0.230238	0.629470	0.676240	0.746388	0.707297	0.897037	0.804932
σ	—	0.0063	—	0.0048	—	0.0016	—	0.0102
B_2	0.007505	0.010751	0.014747	0.01642	0.006686	0.006132	0.005876	0.004847
σ	—	0.0006	—	0.0002	—	0.00004	—	0.0002
σ_f	0.0359	0.0342	0.0267	0.0201	0.0136	0.0089	0.0215	0.0600
Determinant Value	—	$0.5229 \cdot 10^6$	—	$0.1292 \cdot 10^6$	—	$0.2446 \cdot 10^7$	—	$0.6845 \cdot 10^7$

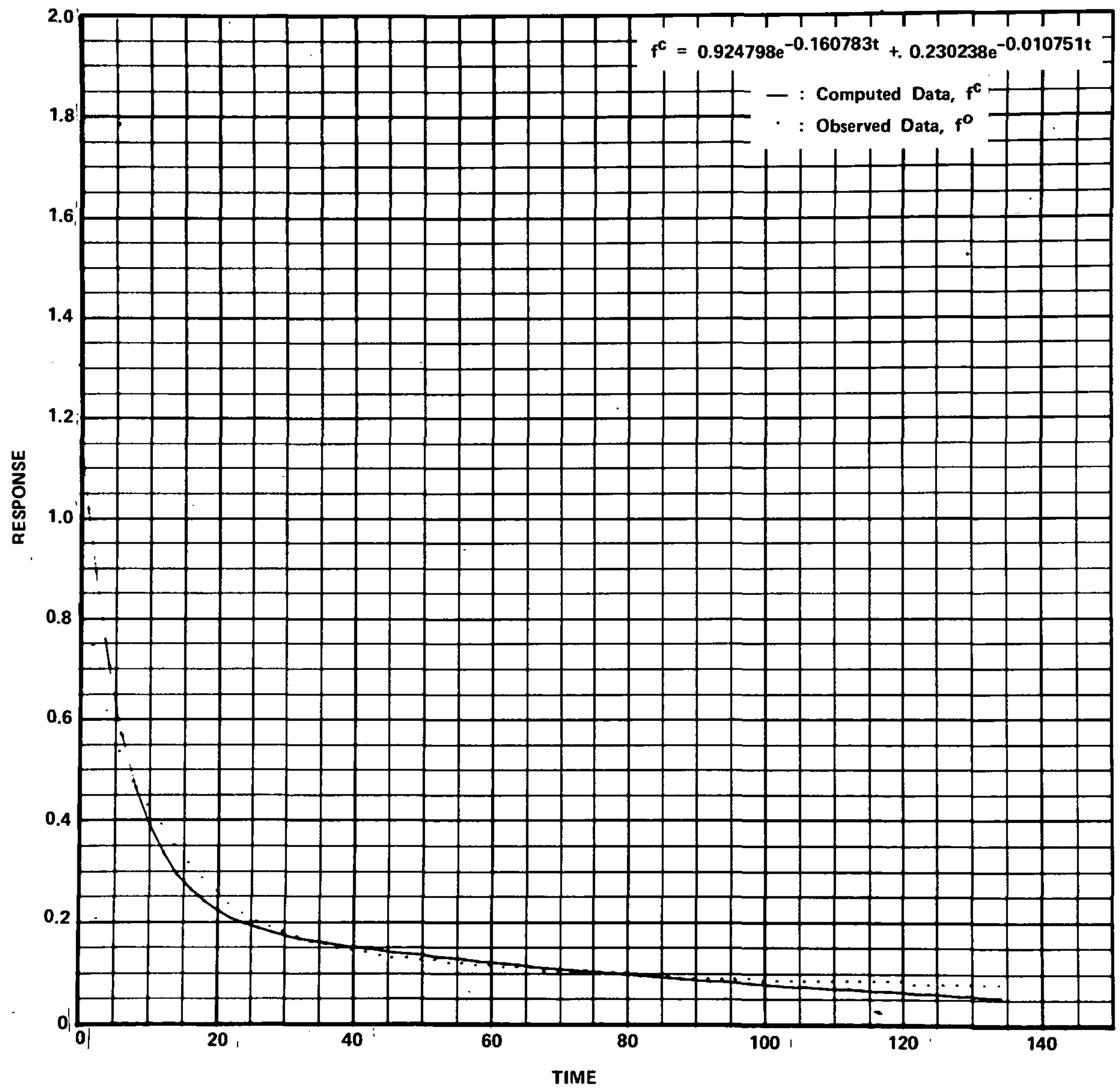

Figure 4. Observed and computed response for Model IV analysis on set 1 data.

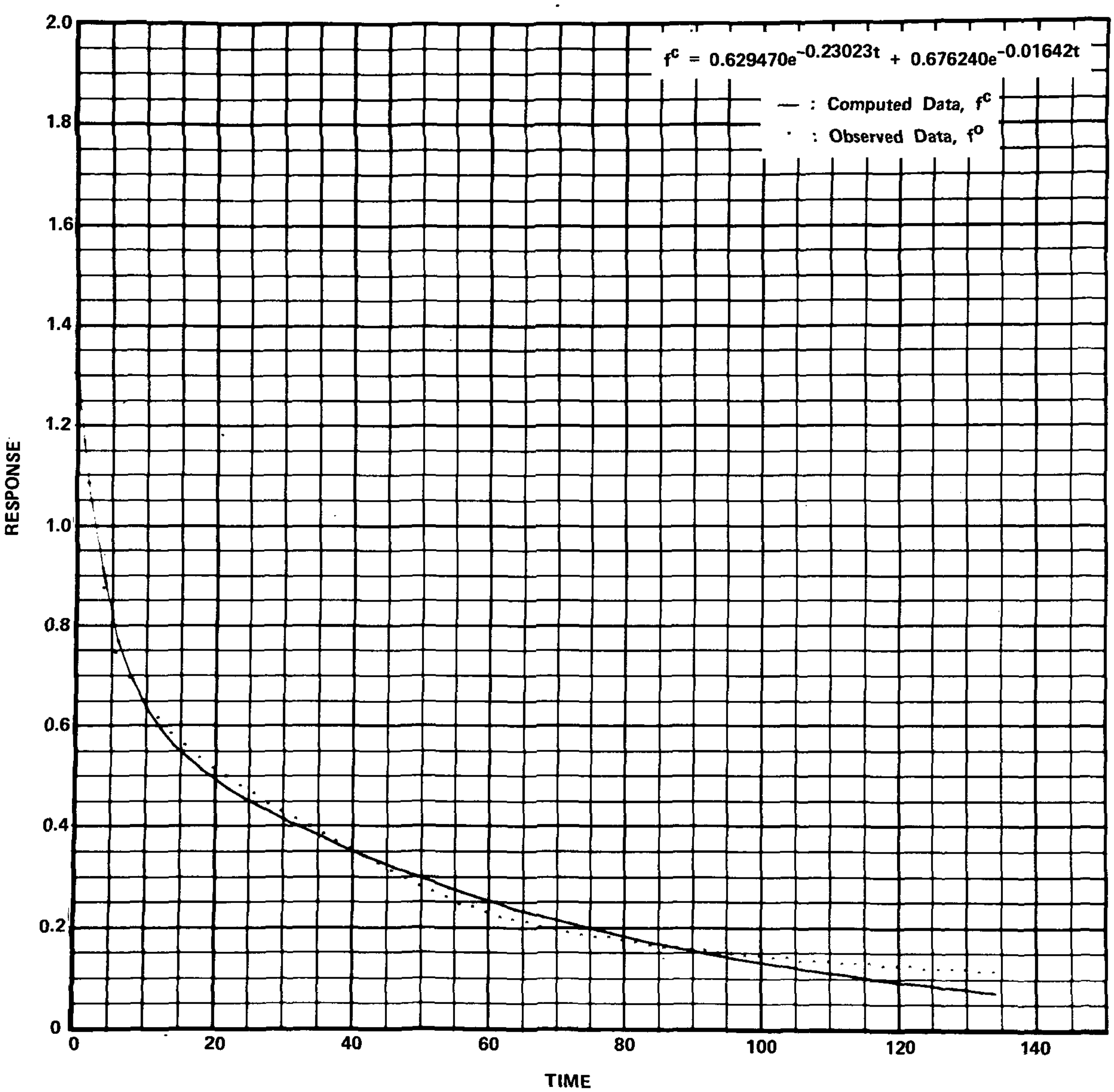

Figure 5. Observed and computed response for Model IV analysis on set 2 data.

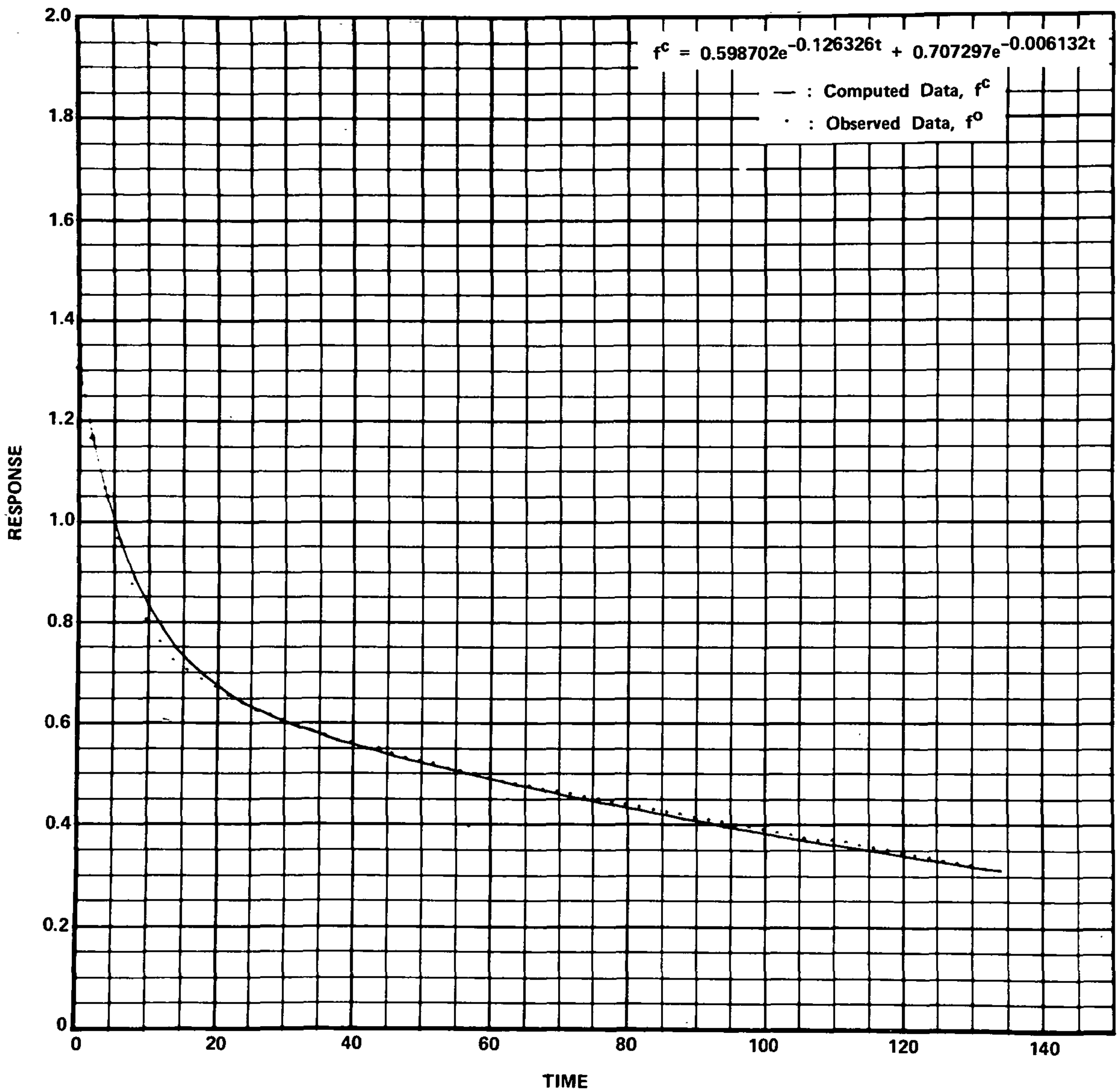

Figure 6. Observed and computed response for Model IV analysis on set 3 data.

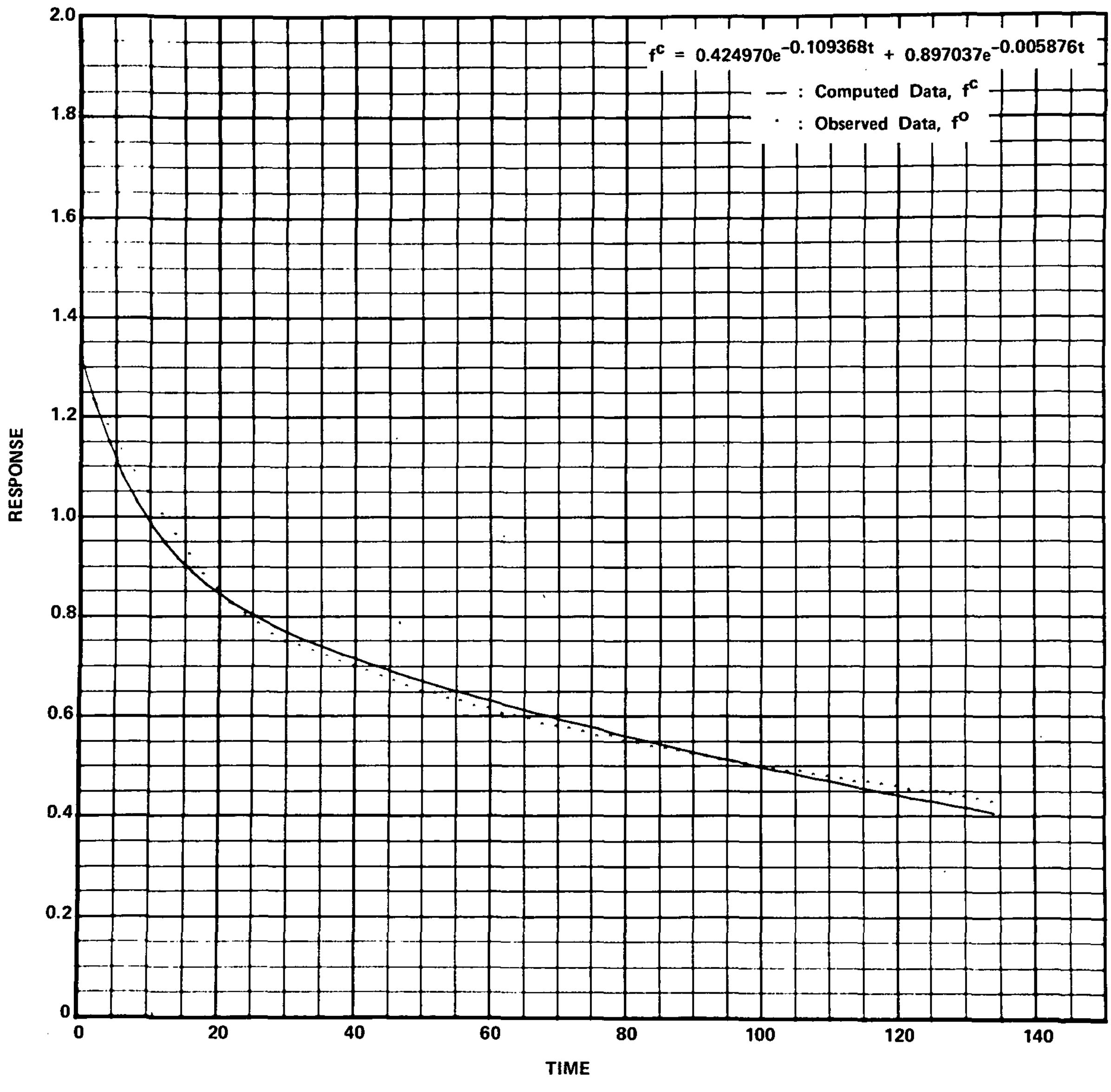

Figure 7. Observed and computed response for Model IV analysis on set 4 data.

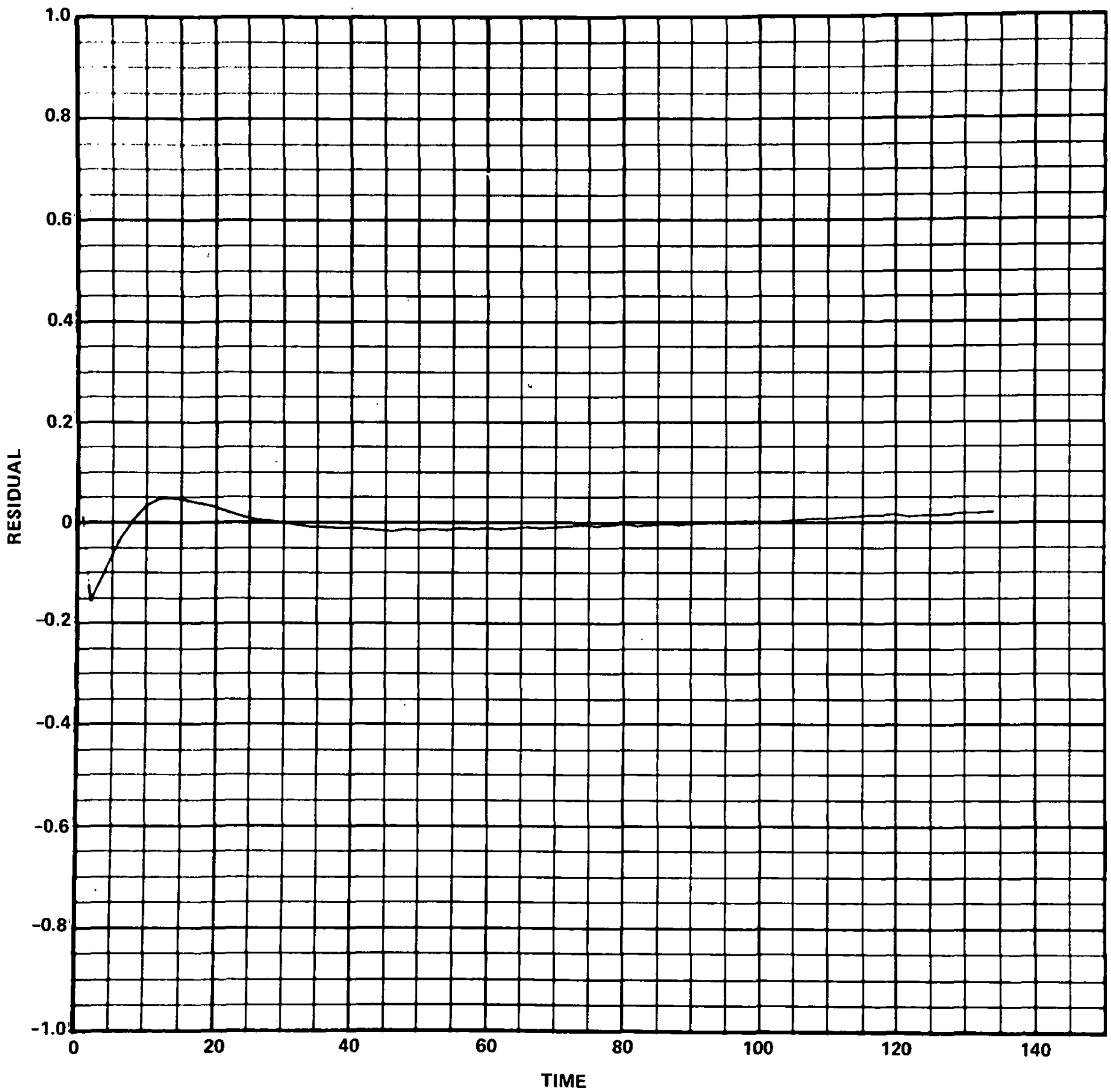

Figure 8. Residuals for Model IV analysis on set 1 data.

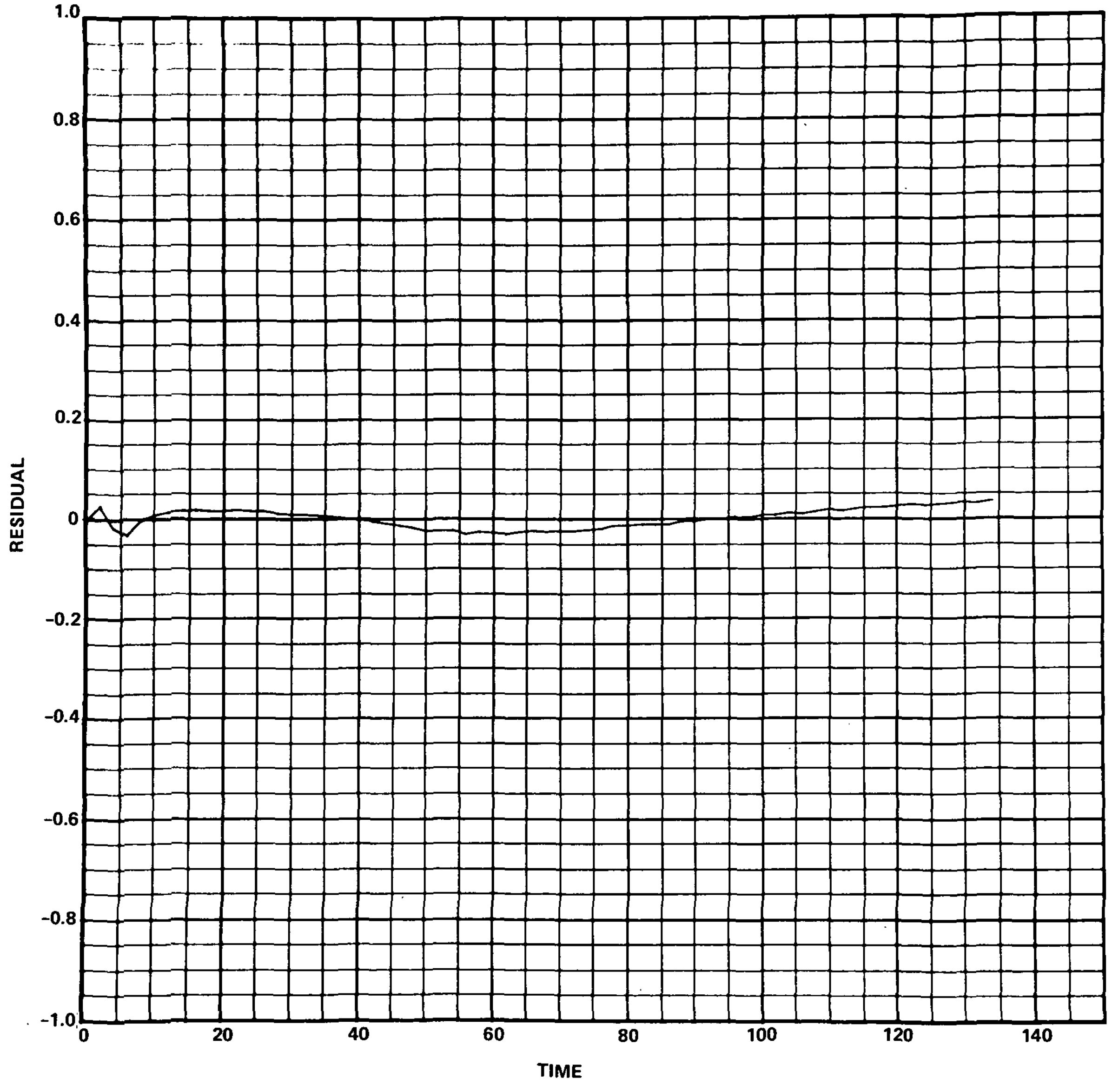

Figure 9. Residuals for Model IV analysis on set 2 data.

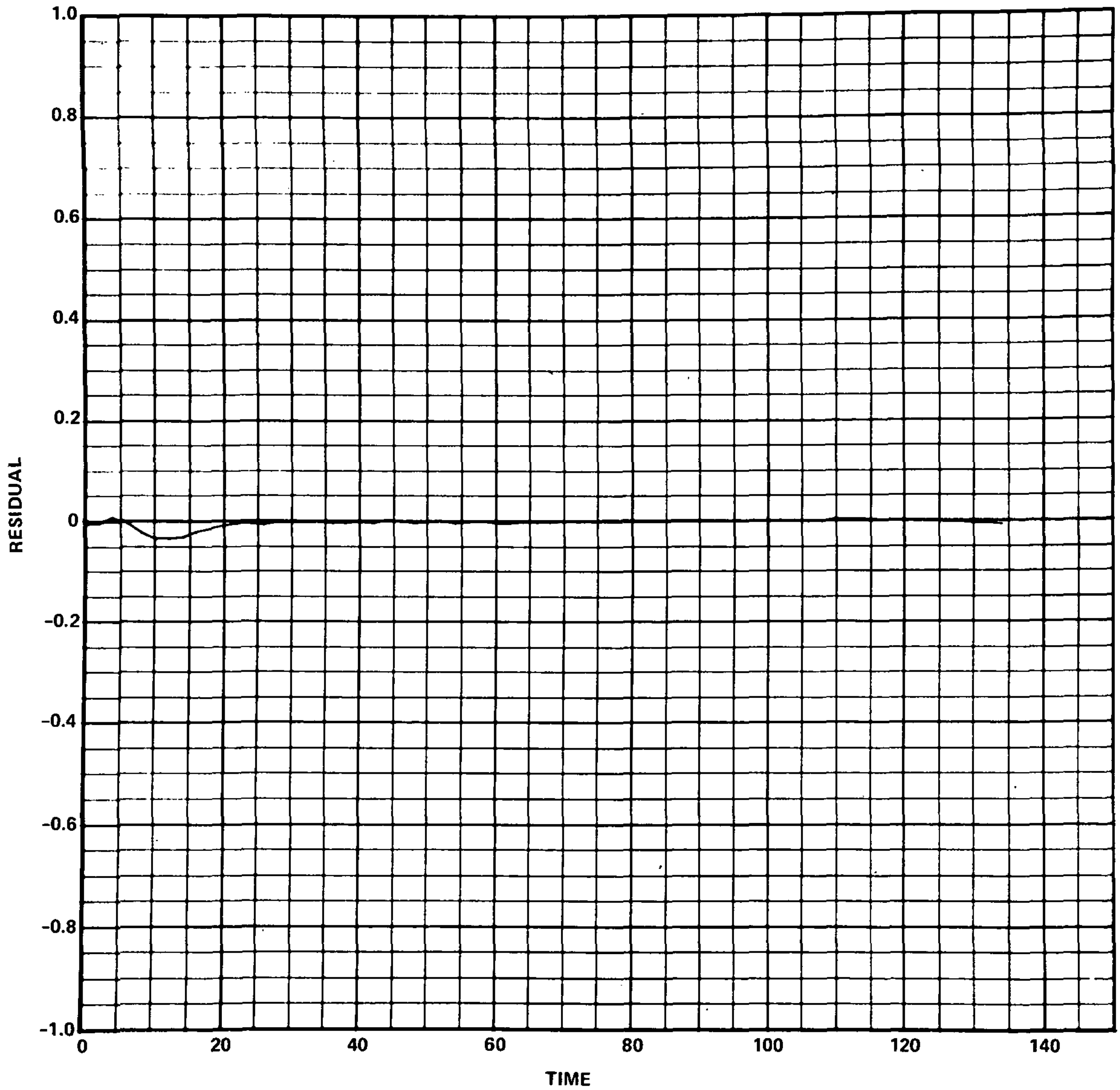

Figure 10. Residuals for Model IV analysis on set 3 data.

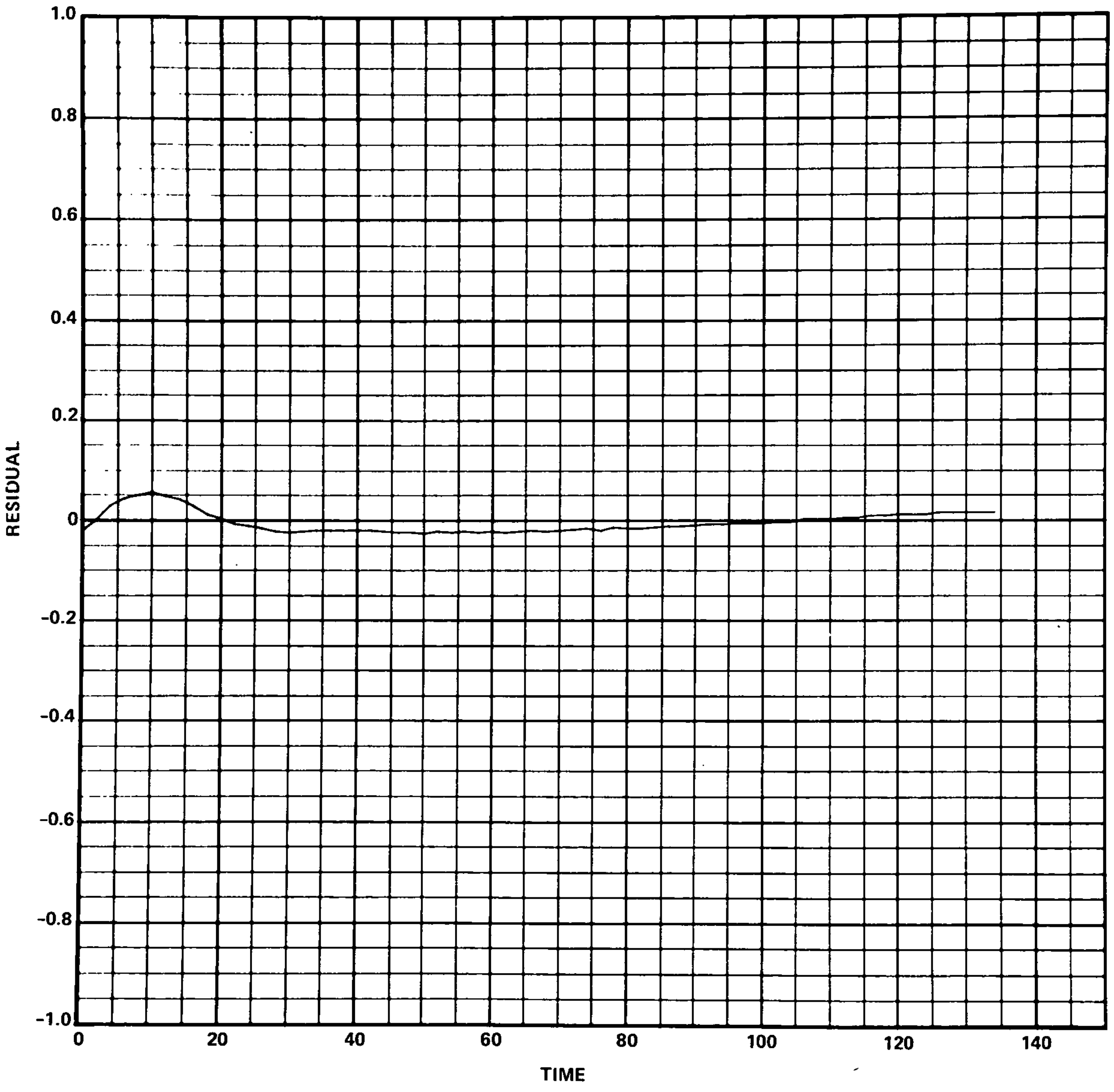

Figure 11. Residuals for Model IV analysis on set 4 data.

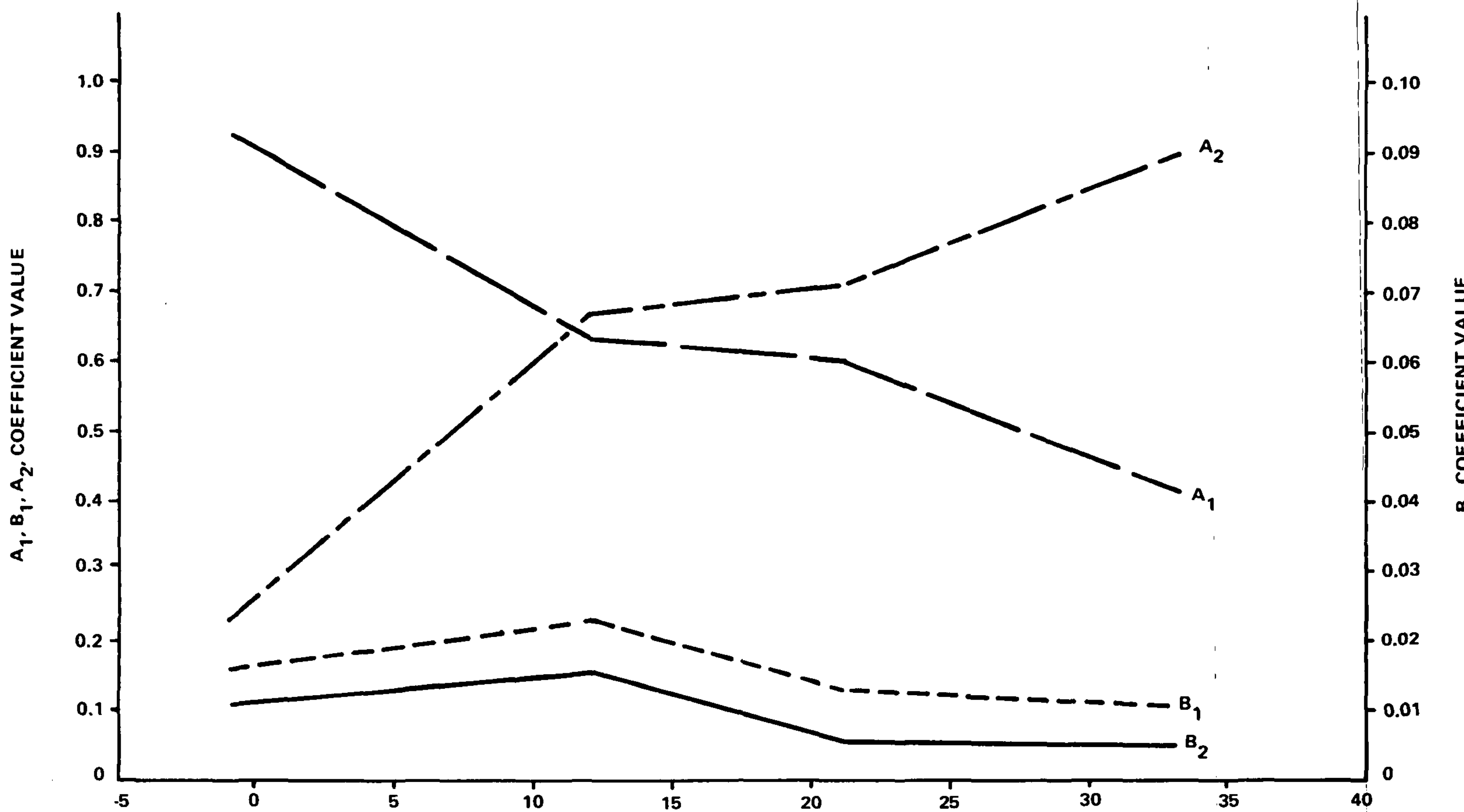

Figure 12. Model IV coefficients versus oxygen evolution time.

APPENDIX

COMPUTER PROGRAM DOCUMENTATION

This appendix presents operational information on the UNIVAC 1108 computer programs concerning the regression analysis application of exponential models to decay-type data. The general organization of the operational version of the two developed programs is depicted in Figure A-1. Since both programs are basically similar, only information concerning Program II is presented. A complete program listing, job card example (Fig. A-2), input preparation, and sample output are included.

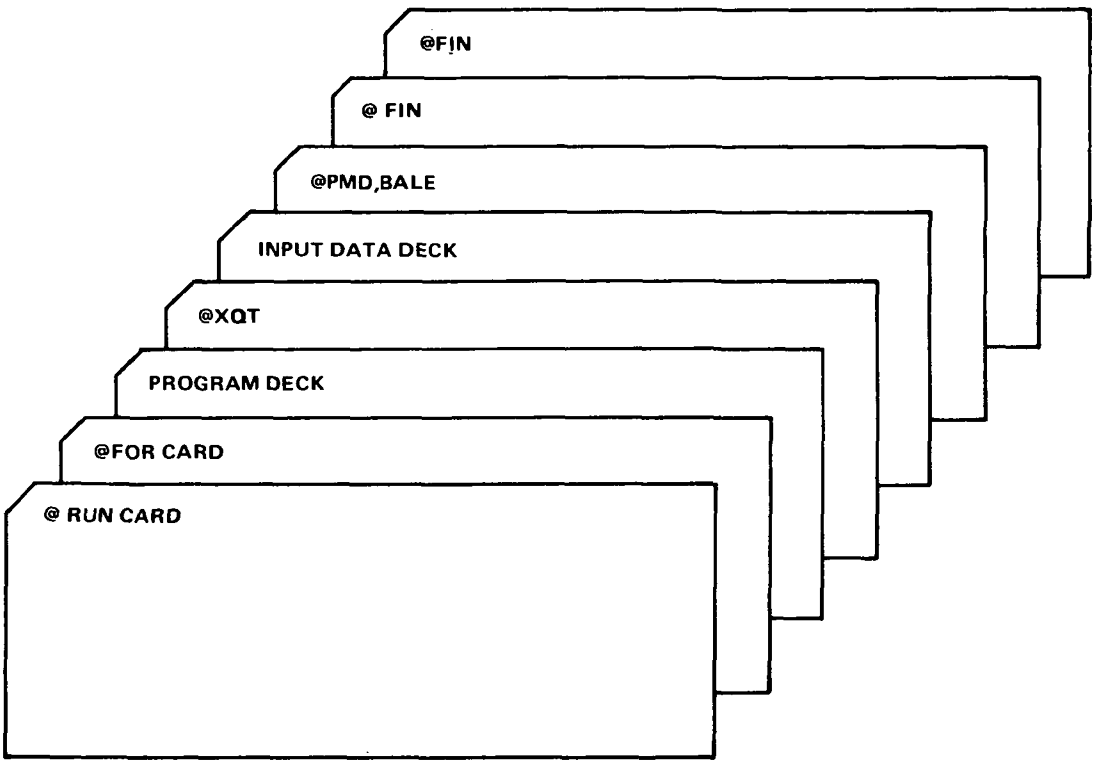

Figure A-1. Program organization.

1108 RUN REQUEST & INSTRUCTIONS

NAME (LAST & INITIAL)	OP CODE	JOB#	PROD #
JUNKIN, B.	12	320600	

BIN#	BLDG#	RM#	RUN-ID	RUN
313	4663	A-217	EXPREG	1 OF 1

EST. CPU RUN TIME	CORE SIZE	PUNCH	
0 HRS. 3 MINS.	24K	N/A	☒ COMPILE ☒ EXECUTE ☐ SORT

	LANGUAGE	MAX. PAGES	☐ SPECIAL FORMS
☐ ☒ EXEC VIII	FOR4	1,500	TYPE COPIES

DOES THIS JOB HAVE A RESTART PROCEDURE? ☐ YES ☐ NO

INPUT TAPES			OUTPUT TAPES ONLY				
REEL NO.	FILE NAME	UNIT	REEL NO.	FILE NAME	LOGIC	UNIT	SAVE

PROGRAMMER COMMENTS:

Set 1 Data: 2 exponentials

☐ OVER

MICRO FILM		COPIES		COPY FLO		OPER. INIT.
#FILES	#FRAMES	P	F	P	F	SEQ.#

OPERATOR COMMENTS: ☐ SEE TECH. ☐ SEE OPER.

MSFC - Form 3019 (Rev August 1969) ☐ OVER

Figure A-2. Job card example.

Description of Data Deck Input Parameters

The card immediately following the @XQT card is the first card of the input data deck. This card specifies the number of cases (NCASES) of data that are to be processed. The format is of the form +XX(13) and appears in columns 1 through 3. The information between the $INPUT card and the $ card is associated with a specific set of data and is input under the non-executable NAMELIST statement. For example, the input statement in the program is

NAMELIST/INPUT/T, Y, NN, TL, TR, YB, YT, YB1, YT1, VARY, TOLER, ITERM4, ITERM3, ITERM2.

The forms that the input data take include variable name and subscripted variable. In the usage above, T and Y are subscripted arrays and the remaining variables are simple variable names. The specific format of the data can be either integer constants (i.e., +218) or real constants (i.e., 1.85921E+00, with or without the E notation). The description of the variables in the NAMELIST statement follows.

T	— array containing the values for the independent variable
Y	— array containing the values for the dependent variable
NN	— number of data points
TL	— left plot limit for the horizontal T axis
TR	— right plot limit for the horizontal T axis
YB	— bottom plot limit for the vertical Y axis
YT	— top plot limit for the vertical Y axis
YB1	— bottom plot limit for vertical residual axis
YT1	— top plot limit for vertical residual axis
VARY	— σ_f^2 , variance for dependent variable
TOLER	— iteration parameter

ITERM4 — control parameter for Model III

ITERM3 — control parameter for Model IV

ITERM2 — control parameter for Model V

Computer Listing of Program II

```
        JJ    UU        UU    NN        NN    KK        KK    IIIIII      NN        NN
        JJ    UU        UU    NNN       NN    KK       KK     IIIIII      NNN       NN
        JJ    UU        UU    NNNN      NN    KK     KK         II        NNNN      NN
        JJ    UU        UU    NNNNN     NN    KK    KK          II        NNNNN     NN
        JJ    UU        UU    NN NNN    NN    KK   KK           II        NN NNN    NN
        JJ    UU        UU    NN  NNN   NN    KK KKK            II        NN  NNN   NN
        JJ    UU        UU    NN   NNN  NN    KKKK KK           II        NN   NNN  NN
        JJ    UU        UU    NN    NNN NN    KK    KK          II        NN    NNN NN
        JJ    UU        UU    NN     NNNNN    KK     KK         II        NN     NNNNN
JJ      JJ    UUU      UUU    NN      NNNN    KK      KK        II        NN      NNNN
 JJJJJJJJJ     UUUUUUUUUU     NN       NNN    KK       KK     IIIIII      NN       NNN
  JJJJJJJ       UUUUUUUU      NN        NN    KK        KK    IIIIII      NN        NN

BBBBBBBBBB      IIIIII        NN        NN      333333          11          333333
BBBBBBBBBBB     IIIIII        NNN       NN    3333333333       111        3333333333
BB       BB       II          NNNN      NN    333      333    1111        333      333
BB       BB       II          NNNNN     NN    33        33      11        33        33
BB       BB       II          NN NNN    NN              33      11                  33
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BBBBBBBBBB        II          NN   NNN  NN             333      11                 333
BB       BB       II          NN    NNN NN              33      11                  33
BB       BB       II          NN     NNNNN    33        33      11        33        33
BB       BB       II          NN      NNNN    333      333      11        333      333
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HVI 009-09/16-13:31 (,0)

MAIN PROGRAM

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EXTERNAL REFERENCES (BLOCK, NAME)

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0004   IDENT
0005   QUIK3L
0006   INVRT
0007   ENDJOB
0010   NINTRS
0011   NRDUS
0012   NIO2$
0013   NWDUS
0014   NWNLS
0015   NWNLS
0016   DLOG
0017   EXP
0020   DEXP
0021   NIO1$
0022   SQRT
0023   DSQRT
0024   NSTOP$

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

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0000  023231 103F   0001  002172 1035G  0000  023240 104F   0001  002206 1043G  0001  002207 1046G
0000  023247 105F   0001  002223 1054G  0000  023266 106F   0001  002241 1061G  0001  002247 1066G
0000  023272 107F   0001  002255 1073G  0000  023277 108F   0000  023317 109F   0000  023326 110F
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0000 I 023026 NN            0000 I 023042 P             0000 D 013134 RES           0000 R 022160 RSS           0000 R 023124 SGA1
0000 R 023126 SGA2          0000 R 023130 SGA3          0000 R 023125 SGB1          0000 R 023127 SGB2          0000 R 023131 SGB3
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0000 R 023132 TOL1          0000 R 023030 TR            0000 R 022324 TS            0000 R 023035 VARY          0000 R 000620 W
0000 D 000764 X1            0000 D 001274 X2            0000 D 001604 X3            0000 D 000310 Y             0000 R 023031 YB
0000 R 023033 YB1           0000 D 013444 YC            0000 R 022634 YCS           0000 R 022470 YS            0000 R 023032 YT
0000 R 023034 YT1
```

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00100       3.    C
00101       4.          DIMENSION T(100),Y(100),A(100),X1(100),X2(100),X3(100),B(100,7),
00101       5.         -BT(7,100),BN(100,1),D1(100,7),D2(7,1),D3(7,7),D(49),DEL(7,1),
00101       6.         -RES(100),YC(100),F(350),AR(7,350),TEMP(100),D33(7,7),DIDEN(7,7),
00101       7.         -BCOT(12),BCDY(12),BCOR(12),DD(36)
00103       8.          DIMENSION RSS(100),TS(100),YS(100),YCS(100)
00104       9.          DOUBLE PRECISION X1,X2,X3,YC,RES,A11,B11,A22,B22,A33,B33,DEL
00105      10.          DOUBLE PRECISION B,BT,BN,D1,D2,D3,D,DD,DETER,D33,DIDEN,T,Y
00106      11.          DOUBLE PRECISION SM1,SM2,SM3,SM4
00107      12.          NAMELIST/INPUT/T,Y,NN,TL,TR,YB,YT,YB1,YT1,VARY,TOLER,ITERM4,
00107      13.         -ITERM3,ITERM2
00110      14.          CALL IDENT(935)
00111      15.          INTEGER P
```

```
00112   100   FORMAT (1H1)
00113   101   FORMAT (///)
00114   102   FORMAT (83H NON-LINEAR EXPONENTIAL REGRESSION ANALYSIS USING AN IT
00114         -ERATIVE CORRECTION PROCEDURE)
00115   103   FORMAT (36H ASSUMED MODEL IS THREE EXPONENTIALS)
00116   104   FORMAT (33H INITIAL ESTIMATES FOR PARAMETERS)
00117   105   FORMAT (3X,3HA1=E13.6,2X,3HB1=E13.6,2X,3HA2=E13.6,2X,3HB2=E13.6,2X
00117         -,3HA3=E13.6,2X,3HB3=E13.6)
00120   106   FORMAT (15H CYCLE NUMBER =I3)
00121   107   FORMAT (3X,22H PARAMETER CORRECTIONS)
00122   108   FORMAT (3X,4HDA1=E13.6,1X,4HDB1=E13.6,1X,4HDA2=E13.6,1X,4HDB2=E13.
00122         -6,1X,4HDA3=E13.6,1X,4HDB3=E13.6)
00123   109   FORMAT (3X,29H IMPROVED PARAMETER ESTIMATES)
00124   110   FORMAT (3X,37H RESPONSE VARIABLE STANDARD DEVIATION)
00125   111   FORMAT (3X,6HSIGY1=E13.6,3X,6HSIGY2=E13.6)
00126   112   FORMAT (3X,31H COEFFICIENT STANDARD DEVIATION)
00127   113   FORMAT (3X,4HSA1=E13.6,1X,4HSB1=E13.6,1X,4HSA2=E13.6,1X,4HSB2=E13.
00127         -6,1X,4HSA3=E13.6,1X,4HSB3=E13.6)
00130   114   FORMAT (3X,6HTOLER=E13.6)
00131   115   FORMAT (3X,5HDTOL=E13.6)
00132   116   FORMAT (3X,29HCONVERGENCE HAS BEEN ACHIEVED)
00133   117   FORMAT (3X,48H VALUES IN LAST CYCLE ARE FINAL PARAMETER VALUES)
00134   118   FORMAT (I3)
00135   119   FORMAT (51H INITIAL ESTIMATES FOR THREE-TERM EXPONENTIAL MODEL)
00136   120   FORMAT (5X,1HI,8X,1HF,14X,2HA1,13X,2HB1,13X,2HA2,13X,2HB2,13X,2HA3
00136         -,13X,2HB3)
00137   121   FORMAT (3X,I3,8(E13.6,2X))
00140   122   FORMAT (3X,31H THE INITIAL ESTIMATES USED ARE)
00141   123   FORMAT (3X,2HI=)
00142   124   FORMAT (49H INITIAL ESTIMATES FOR TWO-TERM EXPONENTIAL MODEL)
00143   125   FORMAT (5X,1HI,8X,1HF,14X,2HA1,13X,2HB1,13X,2HA2,13X,2HB2)
00144   126   FORMAT (3X,I3,6(E13.6,2X))
00145   127   FORMAT (30H INVERSE TIMES ORIGINAL MATRIX)
00146   128   FORMAT (3X,7(E13.6,1X))
00147   129   FORMAT (3X,18H DETERMINANT VALUE)
00150   130   FORMAT (34H ASSUMED MODEL IS TWO EXPONENTIALS)
00151   131   FORMAT (3X,3HA1=E13.6,3X,3HB1=E13.6,3X,3HA2=E13.6,3X,3HB2=E13.6)
00152   132   FORMAT (3X,6HDELA1=E13.6,3X,6HDELB1=E13.6,3X,6HDELA2=E13.6,3X,6HDE
00152         -LB2=E13.6)
00153   133   FORMAT (3X,3HA1=E13.6,3X,3HB1=E13.6,3X,3HA2=E13.6,3X,3HB2=E13.6)
00154   134   FORMAT (3X,5HSGA1=E13.6,3X,5HSGB1=E13.6,3X,5HSGA2=E13.6,3X,5HSGB2=
00154         -E13.6)
00155   135   FORMAT (3X,10H RESIDUALS)
00156   136   FORMAT (3X,E13.6)
00157   137   FORMAT (18H INVERSE OF BT*W*B)
00160   138   FORMAT (9H B MATRIX)
00161   139   FORMAT (51H OBSERVED RESPONSE, COMPUTED RESPONSE AND RESIDUALS)
00162   140   FORMAT (6X,8HOBSERVED,6X,8HCOMPUTED,6X,8HRESIDUAL)
00163   141   FORMAT (21H END OF CYCLE NUMBER I3)
00164   142   FORMAT (76H OBSERVED RESPONSE, COMPUTED RESPONSE, AND RESIDUALS US
00164         -ING INITIAL ESTIMATES)
00165   143   FORMAT (3X,7HSIGYIN=E13.6)
00166   144   FORMAT (7H BT*W*B)
00167   145   FORMAT (33H ASSUMED MODEL IS ONE EXPONENTIAL)
00170   146   FORMAT (20H PARAMETER ESTIMATES)
00171   147   FORMAT (3X,3HA1=E13.6,2X,3HB1=E13.6)
```

```
00172          DATA (BCDT(I),I=1,12)/6HTIME  ,11*6H       /
00174          DATA (BCDY(I),I=1,12)/6HRESPON,6HSE    ,10*6H       /
00176          DATA (BCDR(I),I=1,12)/6HRESIDU,6HAL    ,10*6H       /
00200          READ (5,118) NCASES
00203    200   WRITE (6,100)
00205          READ (5,INPUT)
00210          WRITE (6,INPUT)
00213          IF (ITERM2.NE.0) GO TO 700
00215          IF (ITERM4.EQ.0) GO TO 4000
00215    C
00215    C INITIAL ESTIMATES FOR THREE EXPONENTIALS
00215    C     STRAIGHT LINE FIT TO LOG Y VS. TIME
00215    C
00217          IJ=0
00220          J1=2
00221          BJ1=3.
00222    3000  IJ=IJ+1
00223          SM1=0.
00224          SM2=0.
00225          SM3=0.
00226          SM4=0.
00227          JJ=NN-J1
00230          DO 300 I=JJ,NN
00233          SM1=T(I)**2+SM1
00234          SM2=DLOG(Y(I))+SM2
00235          SM3=T(I)+SM3
00236    300   SM4=T(I)*DLOG(Y(I))+SM4
00240          CAA3=BJ1*SM1-SM3**2
00241          CA3=(SM1*SM2-SM3*SM4)/CAA3
00241    C
00241    C ESTIMATES FOR A3,B3
00241    C
00242          B3=-((BJ1*SM4-SM3*SM2)/CAA3)
00243          A3=EXP(CA3)
00244          J2=J1+3
00244    C
00244    C STRAIGHT LINE FIT TO LOG RESIDUAL VS. TIME
00244    C
00245          JJ=NN-J2
00246          JN=NN-J1-1
00247          SM1=0.
00250          SM2=0.
00251          SM3=0.
00252          SM4=0.
00253          DO 301 I=JJ,JN
00256          X3(I)=-B3*T(I)
00257          RES(I)=Y(I)-A3*DEXP(X3(I))
00260          RES(I)=DABS(RES(I))
00261          SM1=T(I)**2+SM1
00262          SM2=DLOG(RES(I))+SM2
00263          SM3=T(I)+SM3
00264    301   SM4=T(I)*DLOG(RES(I))+SM4
00266          CAA2=3.*SM1-SM3**2
00267          CA2=(SM1*SM2-SM3*SM4)/CAA2
00267    C
00267    C ESTIMATES FOR A2,B2
```

```
00267    C
00270          B2=-((3.*SM4-SM3*SM2)/CAA2)
00271          A2=EXP(CA2)
00271    C
00271    C STRAIGHT LINE FIT TO LOG RESIDUAL VS. TIME
00271    C
00272          JN=NN-J2-1
00273          BJ2=JN
00274          SM1=0.
00275          SM2=0.
00276          SM3=0.
00277          SM4=0.
00300          DO 302 I=1,JN
00303          X3(I)=-B3*T(I)
00304          X2(I)=-B2*T(I)
00305          RES(I)=Y(I)-A2*DEXP(X2(I))-A3*DEXP(X3(I))
00306          RES(I)=DABS(RES(I))
00307          SM1=T(I)**2+SM1
00310          SM2=DLOG(RES(I))+SM2
00311          SM3=T(I)+SM3
00312    302   SM4=T(I)*DLOG(RES(I))+SM4
00314          CAA1=BJ2*SM1-SM3**2
00315          CA1=(SM1*SM2-SM3*SM4)/CAA1
00315    C
00315    C ESTIMATES FOR A1,B1
00315    C
00316          B1=-((BJ2*SM4-SM3*SM2)/CAA1)
00317          A1=EXP(CA1)
00317    C
00317    C WEIGHTED SUM OF SQUARES OF DEVIATIONS,W=1.
00317    C
00320          DO 303 I=1,NN
00323          X1(I)=-B1*T(I)
00324          X2(I)=-B2*T(I)
00325    303   X3(I)=-B3*T(I)
00327          SUMDEV=0.
00330          DO 304 I=1,NN
00333          B(I,1)=DEXP(X1(I))
00334          B(I,3)=DEXP(X2(I))
00335          B(I,5)=DEXP(X3(I))
00336    304   SUMDEV=(Y(I)-A1*B(I,1)-A2*B(I,3)-A3*B(I,5))**2+SUMDEV
00340          J1=J1+1
00341          BJ1=BJ1+1.
00342          KTER=NN-J1-6
00343          F(IJ)=SUMDEV
00344          AR(1,IJ)=A1
00345          AR(2,IJ)=B1
00346          AR(3,IJ)=A2
00347          AR(4,IJ)=B2
00350          AR(5,IJ)=A3
00351          AR(6,IJ)=B3
00352          NKOT=IJ
00353          IF (KTER.EQ.0) GO TO 305
00355          GO TO 3000
00356    305   CONTINUE
00356    C
```

```
00356    C SELECTION OF SMALLEST F AND CORRESPONDING PARAMETERS
00356    C
00357              DO 307 I=1,IJ
00362              IF (F(I).LT.0.) GO TO 306
00364              GO TO 307
00365    306       F(I)=-F(I)
00366    307       CONTINUE
00370              JJ1=1
00371              NKOT=NKOT-1
00372              J=1
00373              K=2
00374              TEMP(1)=F(1)
00375    308       DF=TEMP(J)-F(K)
00376              IF (DF.GT.0.) GO TO 309
00400              K=K+1
00401              JJ1=K-1
00402              NKOT=NKOT-1
00403              IF (NKOT.EQ.0) GO TO 310
00405              GO TO 308
00406    309       J=JJ1+1
00407              TEMP(J)=F(K)
00410              K=K+1
00411              JJ1=K-1
00412              NKOT=NKOT-1
00413              IF (NKOT.EQ.0) GO TO 310
00415              GO TO 308
00416    310       CONTINUE
00417              A1=AR(1,J)
00420              B1=AR(2,J)
00421              A2=AR(3,J)
00422              B2=AR(4,J)
00423              A3=AR(5,J)
00424              B3=AR(6,J)
00425              JSEL3=J
00426              WRITE (6,100)
00430              WRITE (6,101)
00432              WRITE (6,119)
00434              WRITE (6,120)
00436              DO 311 I=1,IJ
00441    311       WRITE (6,121) (I,F(I),(AR(J,I),J=1,6))
00452              WRITE (6,101)
00454              WRITE (6,122)
00456              WRITE (6,123) JSEL3
00461    4000      CONTINUE
00462              IF (ITERM3.EQ.0) GO TO 5000
00462    C
00462    C INITIAL ESTIMATES FOR TWO EXPONENTIALS
00462    C         STRAIGHT LINE FIT TO LOG Y VS. TIME
00462    C
00464              IJ=0
00465              J1=2
00466              BJ1=3.
00467    401       IJ=IJ+1
00470              SM1=0.
00471              SM2=0.
00472              SM3=0.
```

```
00473               SM4=0.
00474               JJ=NN-J1
00475               DO 400 I=JJ,NN
00500               SM1=T(I)**2+SM1
00501               SM2=DLOG(Y(I))+SM2
00502               SM3=T(I)+SM3
00503         400   SM4=T(I)*DLOG(Y(I))+SM4
00505               CAA2=BJ1*SM1-SM3**2
00506               CA2=(SM1*SM2-SM3*SM4)/CAA2
00506         C
00506         C ESTIMATES FOR A2,B2
00506         C
00507               B2=-((BJ1*SM4-SM3*SM2)/CAA2)
00510               A2=EXP(CA2)
00511               J2=J1+3
00511         C
00511         C STRAIGHT LINE FIT TO LOG RESIDUAL VS. TIME
00511         C
00512               JN=NN-J1-1
00513               BJ2=JN
00514               SM1=0.
00515               SM2=0.
00516               SM3=0.
00517               SM4=0.
00520               DO 402 I=1,JN
00523               X2(I)=-B2*T(I)
00524               RES(I)=Y(I)-A2*DEXP(X3(I))
00525               RES(I)=DABS(RES(I))
00526               SM1=T(I)**2+SM1
00527               SM2=DLOG(RES(I))+SM2
00530               SM3=T(I)+SM3
00531         402   SM4=T(I)*DLOG(RES(I))+SM4
00533               CAA1=BJ2*SM1-SM3**2
00534               CA1=(SM1*SM2-SM3*SM4)/CAA1
00534         C
00534         C ESTIMATES FOR A1,B1
00534         C
00535               B1=-((BJ2*SM4-SM3*SM2)/CAA1)
00536               A1=EXP(CA1)
00536         C
00536         C WEIGHTED SUM OF SQUARES OF DEVIATIONS,W=1.
00536         C
00537               DO 403 I=1,NN
00542               X1(I)=-B1*T(I)
00543         403   X2(I)=-B2*T(I)
00545               SUMDEV=0.
00546               DO 404 I=1,NN
00551               B(I,1)=DEXP(X1(I))
00552               B(I,3)=DEXP(X2(I))
00553         404   SUMDEV=(Y(I)-A1*B(I,1)-A2*B(I,3))**2+SUMDEV
00555               J1=J1+1
00556               BJ1=BJ1+1.
00557               KTER=NN-J1-3
00560               F(IJ)=SUMDEV
00561               AR(1,IJ)=A1
00562               AR(2,IJ)=B1
```

```
00563              AR(3,IJ)=A2
00564              AR(4,IJ)=B2
00565              NKOT=IJ
00566              IF (KTER.EQ.0) GO TO 405
00570              GO TO 401
00571        405   CONTINUE
00571        C
00571        C SELECTION OF SMALLEST F AND CORRESPONDING PARAMETERS
00571        C
00572              DO 407 I=1,IJ
00575              IF (F(I).LT.0.) GO TO 406
00577              GO TO 407
00600        406   F(I)=-F(I)
00601        407   CONTINUE
00603              JJ1=1
00604              NKOT=NKOT-1
00605              J=1
00606              K=2
00607              TEMP(1)=F(1)
00610        408   DF=TEMP(J)-F(K)
00611              IF (DF.GT.0.) GO TO 409
00613              K=K+1
00614              JJ1=K-1
00615              NKOT=NKOT-1
00616              IF (NKOT.EQ.0) GO TO 410
00620              GO TO 408
00621        409   J=JJ1+1
00622              TEMP(J)=F(K)
00623              K=K+1
00624              JJ1=K-1
00625              NKOT=NKOT-1
00626              IF (NKOT.EQ.0) GO TO 410
00630              GO TO 408
00631        410   CONTINUE
00632              A1=AR(1,J)
00633              B1=AR(2,J)
00634              A2=AR(3,J)
00635              B2=AR(4,J)
00636              JSEL2=J
00637              WRITE (6,100)
00641              WRITE (6,101)
00643              WRITE (6,124)
00645              WRITE (6,125)
00647              DO 411 I=1,IJ
00652        411   WRITE (6,126) (I,F(I),(AR(J,I),J=1,4))
00663              WRITE (6,101)
00665              WRITE (6,122)
00667              WRITE (6,123) JSEL2
00672        5000  CONTINUE
00672        C
00672        C STATEMENTS NUMBERED 500-599 REFER TO PROGRAM FOR THREE
00672        C     EXPONENTIALS
00672        C
00673              IF (ITERM4.EQ.0) GO TO 600
00675        500   CONTINUE
00675        C
```

```
00675    C THREE EXPONENTIALS
00675    C      ITERM4=1
00675    C
00676           WRITE (6,100)
00700           WRITE (6,102)
00702           WRITE (6,101)
00704           WRITE (6,103)
00706           WRITE (6,104)
00710           WRITE (6,105) A1,B1,A2,B2,A3,B3
00720           KCYCLE=0
00721           A11=A1
00722           B11=B1
00723           A22=A2
00724           B22=B2
00725           A33=A3
00726           B33=B3
00727           BJ=NN
00730           SUMSQ=0.
00731           WRITE (6,142)
00733           WRITE (6,101)
00735           WRITE (6,140)
00737           DO 5001 I=1,NN
00742           X1(I)=-B11*T(I)
00743           X2(I)=-B22*T(I)
00744           X3(I)=-B33*T(I)
00745           B(I,1)=DEXP(X1(I))
00746           B(I,3)=DEXP(X2(I))
00747           B(I,5)=DEXP(X3(I))
00750           YC(I)=A11*B(I,1)+A22*B(I,3)+A33*B(I,5)
00751           RES(I)=Y(I)-YC(I)
00752           RSS(I)=RES(I)
00753           TS(I)=T(I)
00754           YS(I)=Y(I)
00755           YCS(I)=YC(I)
00756           SUMSQ=RES(I)**2+SUMSQ
00757    5001   WRITE (6,128) Y(I),YC(I),RES(I)
00765           SIGYIN=SQRT(SUMSQ/(BJ-6.))
00766           WRITE (6,143) SIGYIN
00771           KK=NN
00772           CALL QUIK3L (-1,TL,TR,YB,YT,43,BCDT,BCDY,KK,TS,YS)
00773           CALL QUIK3L (0,TL,TR,YB,YT,35,BCDT,BCDY,-KK,TS,YCS)
00774           CALL QUIK3L(-1,TL,TR,YB1,YT1,35,BCDT,BCDR,-KK,TS,RSS)
00774    C
00774    C W MATRIX
00774    C
00775           DO 501 I=1,NN
01000    501    W(I)=1./VARY
01000    C
01000    C B MATRIX
01000    C
01002    5010   CONTINUE
01003           KCYCLE=KCYCLE+1
01004           WRITE (6,101)
01006           WRITE (6,106) KCYCLE
01011           DO 502 I=1,NN
01014           X1(I)=-B11*T(I)
```

```
01015              X2(I)=-B22*T(I)
01016      502     X3(I)=-B33*T(I)
01020              WRITE (6,138)
01022              DO 503 I=1,NN
01025              B(I,1)=DEXP(X1(I))
01026              B(I,2)=-A11*T(I)*B(I,1)
01027              B(I,3)=DEXP(X2(I))
01030              B(I,4)=-A22*T(I)*B(I,3)
01031              B(I,5)=DEXP(X3(I))
01032              B(I,6)=-A33*T(I)*B(I,5)
01033      503     WRITE (6,128) (B(I,JB),JB=1,6)
01033      C
01033      C TRANSPOSE OF B MATRIX
01033      C
01042              DO 504 K=1,6
01045              DO 504 I=1,NN
01050      504     BT(K,I)=B(I,K)
01050      C
01050      C N MATRIX
01050      C
01053              DO 505 I=1,NN
01056      505     BN(I,1)=Y(I)-A11*B(I,1)-A22*B(I,3)-A33*B(I,5)
01056      C
01056      C B-TRANSPOSE*W*N
01056      C
01060              DO 506 I=1,NN
01063      506     D1(I,1)=0.0D0
01065              DO 507 N=1,NN
01070      507     D1(N,1)=W(N)*BN(N,1)
01072              DO 508 I=1,6
01075      508     D2(I,1)=0.0D0
01077              DO 509 M=1,6
01102              DO 509 N=1,NN
01105      509     D2(M,1)=BT(M,N)*D1(N,1)+D2(M,1)
01105      C
01105      C B-TRANSPOSE*W*B
01105      C
01110              DO 510 I=1,NN
01113              DO 510 J=1,6
01116      510     D1(I,J)=0.0D0
01121              DO 511 P=1,6
01124              DO 511 N=1,NN
01127      511     D1(N,P)=W(N)*B(N,P)
01132              DO 512 I=1,6
01135              DO 512 J=1,6
01140      512     D3(I,J)=0.0D0
01143              DO 513 M=1,6
01146              DO 513 P=1,6
01151              DO 513 N=1,NN
01154      513     D3(M,P)=BT(M,N)*D1(N,P)+D3(M,P)
01160              WRITE (6,144)
01162              DO 5130 I=1,6
01165      5130    WRITE (6,128) (D3(I,IX),IX=1,6)
01165      C
01165      C INVERSE OF B-TRANSPOSE*W*B
01165      C
```

```
01174               I2=0
01175               DO 514 I=1,6
01200               DO 514 J=1,6
01203               I2=I2+1
01204               D(I2)=D3(J,I)
01205         514   DD(I2)=D3(J,I)
01210               N=6
01211               M=0
01212               CALL INVRT (D,N,M,DETER)
01212         C
01212         C INVERSE MATRIX
01212         C
01213               K1=1
01214               K2=6
01215               K3=6
01216               K4=6
01217               WRITE (6,137)
01221         5140  WRITE (6,128) (D(I),I=K1,K2)
01227               K1=K2+1
01230               K2=K2+K3
01231               K4=K4-1
01232               IF (K4.EQ.0) GO TO 5141
01234               GO TO 5140
01235         5141  CONTINUE
01235         C
01235         C INVERSE*ORIGINAL MATRIX
01235         C
01236               I2=0
01237               DO 515 I=1,6
01242               DO 515 J=1,6
01245               I2=I2+1
01246         515   D33(J,I)=D(I2)
01251               DO 5150 I=1,6
01254               DO 5150 J=1,6
01257         5150  DIDEN(I,J)=0.0D0
01262               DO 5151 M=1,6
01265               DO 5151 P=1,6
01270               DO 5151 N=1,6
01273         5151  DIDEN(M,P)=D33(M,N)*D3(N,P)+DIDEN(M,P)
01277               IW=6
01300               I=1
01301               WRITE (6,127)
01303         5152  WRITE (6,128) (DIDEN(I,J),J=1,6)
01311               IW=IW-1
01312               IF (IW.EQ.0) GO TO 5153
01314               I=I+1
01315               GO TO 5152
01316         5153  CONTINUE
01317               WRITE (6,101)
01321               WRITE (6,129)
01323               WRITE (6,128) DETER
01323         C
01323         C DELTA MATRIX
01323         C
01326               DO 516 I=1,6
01331         516   DEL(I,I)=0.0D0
```

```
01333               DO 517 M=1,6
01336               DO 517 N=1,6
01341         517   DEL(M,1)=D33(M,N)*D2(N,1)+DEL(M,1)
01341         C
01341         C IMPROVED PARAMETER ESTIMATES
01341         C
01344               A11=A11+DEL(1,1)
01345               B11=B11+DEL(2,1)
01346               A22=A22+DEL(3,1)
01347               B22=B22+DEL(4,1)
01350               A33=A33+DEL(5,1)
01351               B33=B33+DEL(6,1)
01351         C
01351         C RESIDUALS USING IMPROVED PARAMETER ESTIMATES
01351         C
01352               DO 519 I=1,NN
01355               X1(I)=-B11*T(I)
01356               X2(I)=-B22*T(I)
01357         519   X3(I)=-B33*T(I)
01361               DO 520 I=1,NN
01364               B(I,1)=DEXP(X1(I))
01365               B(I,3)=DEXP(X2(I))
01366         520   B(I,5)=DEXP(X3(I))
01370               WRITE (6,100)
01372               WRITE (6,139)
01374               WRITE (6,101)
01376               WRITE (6,140)
01400               DO 521 I=1,NN
01403               YC(I)=A11*B(I,1)+A22*B(I,3)+A33*B(I,5)
01404               RES(I)=Y(I)-YC(I)
01405               RSS(I)=RES(I)
01406               YCS(I)=YC(I)
01407         521   WRITE (6,128) Y(I),YC(I),RES(I)
01407         C
01407         C STANDARD DEVIATION OF RESPONSE VARIABLE USING INITIAL ESTIMATES
01407         C
01415               BJ=NN
01416               SUM1=0.
01417               DO 522 I=1,NN
01422         522   SUM1=BN(I,1)**2+SUM1
01424               SIGY1=SQRT(SUM1/(BJ-6.))
01424         C
01424         C STANDARD DEVIATION OF RESPONSE VARIABLE USING IMPROVED ESTIMATES
01424         C
01425               SUM2=0.
01426               DO 523 I=1,NN
01431               SIGY2=SQRT(SUM2/(BJ-6.))
01432         523   SUM2=RES(I)**2+SUM2
01432         C
01432         C PARAMETER STANDARD DEVIATIONS
01432         C
01434               SGA1=SIGY2/SQRT(D3(1,1))
01435               SGB1=SIGY2/SQRT(D3(2,2))
01436               SGA2=SIGY2/SQRT(D3(3,3))
01437               SGB2=SIGY2/SQRT(D3(4,4))
01440               SGA3=SIGY2/SQRT(D3(5,5))
```

```
01441            SGB3=SIGY2/SQRT(D3(6,6))
01442            WRITE (6,101)
01444            WRITE (6,127)
01446            WRITE (6,108) (DEL(I,I),I=1,6)
01454            WRITE (6,101)
01456            WRITE (6,109)
01460            WRITE (6,105) A11,B11,A22,B22,A33,B33
01470            WRITE (6,101)
01472            WRITE (6,110)
01474            WRITE (6,111) SIGY1,SIGY2
01500            WRITE (6,101)
01502            WRITE (6,112)
01504            WRITE (6,113) SGA1,SGB1,SGA2,SGB2,SGA3,SGB3
01504      C
01504      C ITERATION LOGIC CYCLE
01504      C
01514            TOL1=SIGY2**2-SIGY1**2
01515            DTOL=TOLER-TOL1
01516            DTOL=ABS(DTOL)
01517            IF ((DTOL-.00001).GT.0.) GO TO 524
01521            GO TO 525
01522      524   TOLER=TOL1
01523            WRITE (6,101)
01525            WRITE (6,114) TOLER
01530            WRITE (6,141) KCYCLE
01533      525   WRITE (6,101)
01535            WRITE (6,100)
01537            WRITE (6,115) DTOL
01542            WRITE (6,116)
01544            WRITE (6,117)
01546            KK=NN
01547            CALL QUIK3L (-1,TL,TR,YB,YT,43,BCDT,BCDY,KK,TS,YS)
01550            CALL QUIK3L (0,TL,TR,YB,YT,35,BCDT,BCDY,-KK,TS,YCS)
01551            CALL QUIK3L (-1,TL,TR,YB1,YT1,35,BCDT,BCDR,-KK,TS,RSS)
01552            NCASES=NCASES-1
01553            IF (NCASES.EQ.0) GO TO 800
01553      C
01553      C STATEMENTS NUMBERED 600-699 REFER TO PROGRAM FOR TWO
01553      C     EXPONENTIALS
01553      C
01555            IF (ITERM3.EQ.0) GO TO 200
01557      600   CONTINUE
01557      C
01557      C TWO EXPONENTIALS
01557      C     ITERM3=1
01557      C
01560            WRITE (6,100)
01562            WRITE (6,102)
01564            WRITE (6,101)
01566            WRITE (6,130)
01570            WRITE (6,104)
01572            WRITE (6,131) A1,B1,A2,B2
01600            KCYCLE=0
01601            A11=A1
01602            B11=B1
01603            A22=A2
```

```
01604          B22=B2
01605          BJ=NN
01606          SUMSQ=0.
01607          WRITE (6,142)
01611          WRITE (6,101)
01613          WRITE (6,140)
01615          DO 6001 I=1,NN
01620          X1(I)=-B11*T(I)
01621          X2(I)=-B22*T(I)
01622          B(I,1)=DEXP(X1(I))
01623          B(I,3)=DEXP(X2(I))
01624          YC(I)=A11*B(I,1)+A22*B(I,3)
01625          RES(I)=Y(I)-YC(I)
01626          RSS(I)=RES(I)
01627          TS(I)=T(I)
01630          YS(I)=Y(I)
01631          YCS(I)=YC(I)
01632          SUMSQ=RES(I)**2+SUMSQ
01633    6001  WRITE (6,128) Y(I),YC(I),RES(I)
01641          SIGYIN=SQRT(SUMSQ/(BJ-4.))
01642          WRITE (6,143) SIGYIN
01645          KK=NN
01646          CALL QUIK3L (-1,TL,TR,YB,YT,43,BCDT,BCDY,KK,TS,YS)
01647          CALL QUIK3L (0,TL,TR,YB,YT,35,BCDT,BCDY,-KK,TS,YCS)
01650          CALL QUIK3L(-1,TL,TR,YB1,YT1,35,BCDT,BCDR,-KK,TS,RSS)
01650    C
01650    C W MATRIX
01650    C
01651          DO 601 I=1,NN
01654    601   W(I)=1./VARY
01654    C
01654    C B MATRIX
01654    C
01656    6010  CONTINUE
01657          KCYCLE=KCYCLE+1
01660          WRITE (6,101)
01662          WRITE (6,106) KCYCLE
01665          DO 602 I=1,NN
01670          X1(I)=-B11*T(I)
01671    602   X2(I)=-B22*T(I)
01673          WRITE (6,138)
01675          DO 603 I=1,NN
01700          B(I,1)=DEXP(X1(I))
01701          B(I,2)=-A11*T(I)*B(I,1)
01702          B(I,3)=DEXP(X2(I))
01703          B(I,4)=-A22*T(I)*B(I,3)
01704    603   WRITE (6,128) (B(I,JB),JB=1,4)
01704    C
01704    C TRANSPOSE OF B MATRIX
01704    C
01713          DO 604 K=1,4
01716          DO 604 I=1,NN
01721    604   BT(K,I)=B(I,K)
01721    C
01721    C N MATRIX
01721    C
```

```
01724                 DO 605 I=1,NN
01727         605     BN(I,1)=Y(I)-A11*B(I,1)-A22*B(I,3)
01727         C
01727         C B-TRANSPOSE*W*N
01727         C
01731                 DO 606 I=1,NN
01734         606     D1(I,1)=0.0D0
01736                 DO 607 N=1,NN
01741         607     D1(N,1)=W(N)*BN(N,1)
01743                 DO 608 I=1,4
01746         608     D2(I,1)=0.0D0
01750                 DO 609 M=1,4
01753                 DO 609 N=1,NN
01756         609     D2(M,1)=BT(M,N)*D1(N,1)+D2(M,1)
01756         C
01756         C B-TRANSPOSE*W*B
01756         C
01761                 DO 610 I=1,NN
01764                 DO 610 J=1,4
01767         610     D1(I,J)=0.0D0
01772                 DO 611 P=1,4
01775                 DO 611 N=1,NN
02000         611     D1(N,P)=W(N)*B(N,P)
02003                 DO 612 I=1,4
02006                 DO 612 J=1,4
02011         612     D3(I,J)=0.0D0
02014                 DO 613 M=1,4
02017                 DO 613 P=1,4
02022                 DO 613 N=1,NN
02025         613     D3(M,P)=BT(M,N)*D1(N,P)+D3(M,P)
02031                 WRITE (6,144)
02033                 DO 6130 I=1,4
02036         6130    WRITE (6,128) (D3(I,IX),IX=1,4)
02036         C
02036         C INVERSE OF B-TRANSPOSE*W*B
02036         C
02045                 I2=1
02046                 DO 614 I=1,4
02051                 DO 614 J=1,4
02054                 D(I2)=D3(J,I)
02055         614     I2=I2+1
02060                 N=4
02061                 M=0
02062                 CALL INVRT (D,N,M,DETER)
02062         C
02062         C INVERSE MATRIX
02062         C
02063                 K1=1
02064                 K2=4
02065                 K3=4
02066                 K4=4
02067                 WRITE (6,137)
02071         6140    WRITE (6,128) (D(I),I=K1,K2)
02077                 K1=K2+1
02100                 K2=K2+K3
02101                 K4=K4-1
```

```
02102              IF (K4.EQ.0) GO TO 6141
02104              GO TO 6140
02105      6141    CONTINUE
02106              I2=0
02107              DO 615 I=1,4
02112              DO 615 J=1,4
02115              I2=I2+1
02116      615     D33(J,I)=D(I2)
02116      C
02116      C INVERSE*ORIGINAL MATRIX
02116      C
02121              DO 6150 I=1,4
02124              DO 6150 J=1,4
02127      6150    DIDEN(I,J)=0.0D0
02132              DO 6151 M=1,4
02135              DO 6151 P=1,4
02140              DO 6151 N=1,4
02143      6151    DIDEN(M,P)=D33(M,N)*D3(N,P)+DIDEN(M,P)
02147              IW=4
02150              I=1
02151              WRITE (6,127)
02153      6152    WRITE (6,128) (DIDEN(I,J),J=1,4)
02161              IW=IW-1
02162              IF (IW.EQ.0) GO TO 6153
02164              I=I+1
02165              GO TO 6152
02166      6153    CONTINUE
02167              WRITE (6,101)
02171              WRITE (6,129)
02173              WRITE (6,128) DETER
02173      C
02173      C DELTA MATRIX
02173      C
02176              DO 616 I=1,4
02201      616     DEL(I,1)=0.0D0
02203              DO 617 M=1,4
02206              DO 617 N=1,4
02211      617     DEL(M,1)=D33(M,N)*D2(N,1)+DEL(M,1)
02211      C
02211      C IMPROVED PARAMETER ESTIMATES
02211      C
02214              A11=A11+DEL(1,1)
02215              B11=B11+DEL(2,1)
02216              A22=A22+DEL(3,1)
02217              B22=B22+DEL(4,1)
02217      C
02217      C RESIDUALS USING IMPROVED PARAMETER ESTIMATES
02217      C
02220              DO 619 I=1,NN
02223              X1(I)=-B11*T(I)
02224      619     X2(I)=-B22*T(I)
02226              DO 620 I=1,NN
02231              B(I,1)=DEXP(X1(I))
02232      620     B(I,3)=DEXP(X2(I))
02234              WRITE (6,100)
02236              WRITE (6,139)
```

```
02240         WRITE (6,101)
02242         WRITE (6,140)
02244         DO 621 I=1,NN
02247         YC(I)=A11*B(I,1)+A22*B(I,3)
02250         RES(I)=Y(I)-YC(I)
02251         RSS(I)=RES(I)
02252         YCS(I)=YC(I)
02253   621   WRITE (6,128) Y(I),YC(I),RES(I)
02253   C
02253   C STANDARD DEVIATION OF RESPONSE VARIABLE USING INITIAL ESTIMATES
02253   C
02261         BJ=NN
02262         SUM1=0.
02263         DO 622 I=1,NN
02266   622   SUM1=BN(I,1)**2+SUM1
02270         SIGY1=SQRT(SUM1/(BJ-4.))
02270   C
02270   C STANDARD DEVIATION OF RESPONSE VARIABLE USING IMPROVED ESTIMATES
02270   C
02271         SUM2=0.
02272         DO 623 I=1,NN
02275   623   SUM2=RES(I)**2+SUM2
02277         SIGY2=SQRT(SUM2/(BJ-5.))
02277   C
02277   C PARAMETER STANDARD DEVIATIONS
02277   C
02300         SGA1=SIGY2/SQRT(D3(1,1))
02301         SGB1=SIGY2/SQRT(D3(2,2))
02302         SGA2=SIGY2/SQRT(D3(3,3))
02303         SGB2=SIGY2/SQRT(D3(4,4))
02304         WRITE (6,101)
02306         WRITE (6,107)
02310         WRITE (6,132) (DEL(I,1),I=1,4)
02316         WRITE (6,101)
02320         WRITE (6,109)
02322         WRITE (6,133) A11,B11,A22,B22
02330         WRITE (6,101)
02332         WRITE (6,110)
02334         WRITE (6,111) SIGY1,SIGY2
02340         WRITE (6,101)
02342         WRITE (6,112)
02344         WRITE (6,134) SGA1,SGB1,SGA2,SGB2
02344   C
02344   C ITERATION LOGIC CYCLE
02344   C
02352         TOL1=SIGY2**2-SIGY1**2
02353         DTOL=TOLER-TOL1
02354         DTOL=ABS(DTOL)
02355         IF ((DTOL-.00001).GT.0.) GO TO 624
02357         GO TO 625
02360   624   TOLER=TOL1
02361         WRITE (6,101)
02363         WRITE (6,114) TOLER
02366         WRITE (6,141) KCYCLE
02371         WRITE (6,100)
02373   625   WRITE (6,101)
```

```
02375          WRITE (6,115) DTOL
02400          WRITE (6,116)
02402          WRITE (6,117)
02404          KK=NN
02405          CALL QUIK3L (-1,TL,TR,YB,YT,43,BCDT,BCDY,KK,TS,YS)
02406          CALL QUIK3L (0,TL,TR,YB,YT,35,BCDT,BCDY,-KK,TS,YCS)
02407          CALL QUIK3L(-1,TL,TR,YB1,YT1,35,BCDT,BCDR,-KK,TS,RSS)
02410          NCASES=NCASES-1
02411          IF (NCASES.EQ.0) GO TO 800
02413          GO TO 200
02413    C
02413    C   STATEMENTS NUMBERED 700-799 REFER TO PROGRAM FOR ONE EXPONENTIAL
02413    C    ITERM2=1
02413    C
02413    C
02414    700   SM1=0.0D0
02415          SM2=0.0D0
02416          SM3=0.0D0
02417          SM4=0.0D0
02420          BJ1=NN
02421          SUMSQ=0.
02422          DO 701 I=1,NN
02425          SM1=T(I)**2+SM1
02426          SM2=DLOG(Y(I))+SM2
02427          SM3=T(I)+SM3
02430    701   SM4=T(I)*DLOG(Y(I))+SM4
02432          CAA1=BJ1*SM1-SM3**2
02433          CA1=(SM1*SM2-SM3*SM4)/CAA1
02434          B11=-((BJ1*SM4-SM3*SM2)/CAA1)
02435          A11=DEXP(CA1)
02436          WRITE (6,100)
02440          WRITE (6,145)
02442          WRITE (6,146)
02444          WRITE (6,147) A11,B11
02450          WRITE (6,139)
02452          WRITE (6,101)
02454          WRITE (6,140)
02456          DO 702 I=1,NN
02461          X1(I)=-B11*T(I)
02462          B(I,1)=DEXP(X1(I))
02463          YC(I)=A11*B(I,1)
02464          RES(I)=Y(I)-YC(I)
02465          RSS(I)=RES(I)
02466          TS(I)=T(I)
02467          YS(I)=Y(I)
02470          YCS(I)=YC(I)
02471          SUMSQ=RES(I)**2+SUMSQ
02472    702   WRITE (6,128) Y(I),YC(I),RES(I)
02500          SIGYIN=SQRT(SUMSQ/(BJ1-2.))
02501          WRITE(6,143) SIGYIN
02504          KK=NN
02505          CALL QUIK3L (-1,TL,TR,YB,YT,43,BCDT,BCDY,KK,TS,YS)
02506          CALL QUIK3L (0,TL,TR,YB,YT,35,BCDT,BCDY,-KK,TS,YCS)
02507          CALL QUIK3L (-1,TL,TR,YB1,YT1,35,BCDT,BCDR,-KK,TS,RSS)
02510          NCASES=NCASES-1
02511          IF (NCASES.EQ.0) GO TO 800
```

```
02513    912*          GO TO 200
02514    913*     800  CALL ENDJOB
02515    914*          STOP
02516    915*          END
```

END OF COMPILATION: NO DIAGNOSTICS.

```
@FOR,IS INVRT,INVRT
NVI 009-09/16-13:32 (,0)

   SUBROUTINE INVRT     ENTRY POINT 000365

   STORAGE USED: CODE(1) 000413; DATA(0) 000144; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   TRACSF
    0004   NERR3$

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

    0001   000016 111G     0001   000146 115L     0001   000027 117G     0001   000034 123G     0001   000042 131G
    0001   000116 157G     0001   000255 161L     0001   000163 201G     0001   000203 207G     0001   000225 220G
    0001   000263 234G     0001   000333 235L     0001   000307 245G     0001   000343 250L     0001   000345 255L
    0001   000071 75L      0001   000073 76L      0000 D 000002 AMAX     0000 I 000103 I        0000 I 000106 IC
    0000 I 000104 IND      0000 I 000030 INDEX    0000 I 000110 IND2     0000   000116 INJP$    0000 I 000004 IPIV
    0000 I 000105 IR       0000 I 000100 J        0000 I 000102 K        0000 I 000107 L        0000 I 000101 NN
    0000 D 000000 SIGN


00101                SUBROUTINE INVRT(A,N,M,DETER)
00103                PARAMETER IDIM=20
00103       C        MATRIX INVERSION AND SIMULTANEOUS EQUATIONS SOLVER
00103       C        A=INPUT MATRIX FOR INVERISON OR AUGUMENTED MATRIX FOR SIME. EQS.  IGS00030
00103       C        N=ORDER OF COEFFICIENT MATRIX                                     IGS00040
00103       C        M=0 FOR INVERISON ONLY
00103       C        M=NUMBER OF CONSTANT VECTORS
00103       C        DETER=DETERMINANT OF COEFFICIENT MATRIX
00104                DOUBLE PRECISION A(1),DETER,SIGN,AMAX
00105                DIMENSION IPIV(IDIM),INDEX(IDIM,2)
00106                DETER=1.0D0
00107                SIGN=1.0D0
00110                DO 20 J=1,N
00113             20 IPIV(J)=0
00115                NN=N+M
00116                DO 182 K=1,N
00121                AMAX=0.0D0
00122             45 DO 76 I=1,N
00125                IF (IPIV(I)-1)50,76,50
00130             50 DO 75 J=1,N
00133                IF (IPIV(J)-1)55,75,250
00136             55 IND=(J-1)*N+I
00137                IF(AMAX-DABS(A(IND))) 60,75,75
00142             60 IR=I
00143                IC=J
00144                AMAX=DABS(A(IND))
00145             75 CONTINUE
```

```
00147         76 CONTINUE
00151            IPIV(IC)=IPIV(IC)+1
00152            IF (IR-IC)90,115,90
00155         90 SIGN=-SIGN
00156            DO 110 L=1,NN
00161            IND=(L-1)*N+IR
00162            IND2=(L-1)*N+IC
00163            AMAX=A(IND)
00164            A(IND)=A(IND2)
00165        110 A(IND2)=AMAX
00167        115 INDEX(K,1)=IR
00170            INDEX(K,2)=IC
00171            IND=(IC-1)*N+IC
00172            AMAX=A(IND)
00173            DETER=DETER*AMAX
00174            IF (DETER)140,255,140
00177        140 A(IND)=1.0D0
00200            DO 150 L=1,NN
00203            IND=(L-1)*N+IC
00204        150 A(IND)=A(IND)/AMAX
00206            DO 181 L=1,N
00211            IF (L-IC)165,181,165
00214        165 IND=(IC-1)*N+L
00215            AMAX=A(IND)
00216            A(IND)=0.0D0
00217            DO 180 I=1,NN
00222            IND=(I-1)*N+L
00223            IND2=(I-1)*N+IC
00224            A(IND)=A(IND)-A(IND2)*AMAX
00225        180 CONTINUE
00227        181 CONTINUE
00231        182 CONTINUE
00233            DO 235 I=1,N
00236            L=N+1-I
00237            IR=INDEX(L,1)
00240            IC=INDEX(L,2)
00241            IF (IR-IC)210,235,210
00244        210 DO 230 K=1,N
00247            IND=(IR-1)*N+K
00250            IND2=(IC-1)*N+K
00251            AMAX=A(IND)
00252            A(IND)=A(IND2)
00253        230 A(IND2)=AMAX
00255        235 CONTINUE
00257            DETER=SIGN*DETER
00260            RETURN
00261        250 M=-1
00262        255 RETURN
00263            END

      END OF COMPILATION:          NO   DIAGNOSTICS.
```

```
@FOR,IS DMATML,DMATML
HVI CC9-09/16-13:32 (,0)

   SUBROUTINE DMATML     ENTRY POINT 000160

   STORAGE USED: CODE(1) 000176; DATA(0) 000053; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003    TRACSF
    0004    NERR3$

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

    0001     000034 1L        0001     000061 130G      0001     000067 135G      0001     000102 143G      0001     000035 2L
    0001     000046 3L        0001     000052 4L        0000 D 000000 CD        0000 I 000005 IA1       0000 I 000006 IA2
    0000 I 000002 IA3       0000 I 000007 IB1       0000 I 000010 IB2       0000 I 000013 IB3       0000 I 000003 IM
    0000 I 000004 IN        0000     000022 INJP$     0000 I 000015 LA        0000 I 000016 LB        0000 I 000012 LC
    0000 I 000011 LM        0000 I 000017 LN        0000 I 000014 LP


00101            SUBROUTINE DMATML(C,A,B,M,N,K)
00101      C*    ABSTRACT
00101      C     GENERAL MATRIX MULTIPLICATION ROUTINE  WITH TRANSPOSE OPTIONS
00101      C      WHERE, M IS THE NUMBER OF ROWS OF (A)
00101      C             N IS THE NUMBER OF ROWS OF (B)
00101      C             K IS THE NUMBER OF COLUMNS OF (B) OR (B)T
00101      C     TRANSPOSE OPTIONS ARE CONTROLLED BY THE SIGNS OF M AND N.
00101      C     THE FOLLOWING PRODUCTS MAY BE OBTAINED
00101      C      (C)=(A)(B)        M AND N POSITIVE
00101      C      (C)=(A)T(B)       M NEGATIVE FOR (A)T
00101      C      (C)=(A)(B)T       N NEGATIVE FOR (B)T
00101      C      (C)=(A)T(B)T     M AND N NEGATIVE
00101      C      WHERE T INDICATES TRANSPOSE
00101      C      IF M IS NEGATIVE, M IS THE NUMBER OF ROWS OF (A)T
00101      C      IF N IS NEGATIVE, N IS THE NUMBER OF ROWS OF (B)T
00101      C
00101      C*    OUTPUT ARGUMENT * C
00103            DIMENSION C(1)
00103      C
00103      C*    INPUT ARGUMENTS * A,B,M,N,K
00104            DIMENSION A(1),B(1)
00104      C
00104      C****************************************************************
00105            DOUBLE PRECISION CD,C,A,B
00106            IA3=1
00107            IM=IABS(M)
00110            IN=IABS(N)
00111            IF(M .LT. 0)GO TO 1
00113            IA1=IM
```

```
00114           IA2=1
00115           GO TO 2
00116     1     IA1 = 1
00117           IA2=IN
00120     2     IF(N .LT. 0)GO TO 3
00122           IB1=1
00123           IB2=IN
00124           GO TO 4
00125     3     IB1=K
00126           IB2=1
00127     4     DO 7 LM=1,IM
00132           LC=LM
00133           IB3=1
00134           DO 6 LP=1,K
00137           CD = 0.0D0
00140           LA=IA3
00141           LB=IB3
00142           DO 5 LN=1,IN
00145           CD = CD + A(LA)*B(LB)
00146           LA=LA+IA1
00147     5     LB=LB+IB1
00151           C(LC) = CD
00152           LC = LC + IM
00153     6     IB3=IB3+IB2
00155     7     IA3=IA3+IA2
00157           RETURN
00160           END

        END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MAP,IS EXPO
MAP 17M1-09/16-13:33 -(,0)

    1.      LIB SYS$*MSFC$.

    2.      IN LQCEXP

H$MONITOR     ENTRY POINT     TRACE         ALREADY DEFINED




ADDRESS LIMITS     001000 037532      040000 076226
STARTING ADDRESS   031714

WORDS DECIMAL       15707 IBANK        15511 DBANK



               SEGMENT MAIN            001000 037532      040000 076226

NSWTC$/FOR              1    001000 001021
NRBLK$/MSFC55           1    001022 001110       0    040000 040001
NRWND$/FOR50            1    001111 001170       2    040002 040013
NWEF$/MSFC55            1    001171 001425       2    040014 040034
NEXP6$/MSFC57           1    001426 001620       2    040035 040106
ALOG$/FOR51             1    001621 001736       2    040107 040147
CSIG6V/SC4020           1    001737 002225       0    040150 040206
                                                 2    BLANK$COMMON
CERMRK/SC4020           1    002226 002255       0    040207 040222
                                                 2    BLANK$COMMON
CLABLV/SC4020           1    002256 003315       0    040223 040331
                                                 2    BLANK$COMMON
NFTCH$/FOR57            1    003316 003615       2    040332 040367
NFTV$/FOR               1    003616 003640
NCLOS$/MSFC57           1    003641 004007       2    040370 040415
NWBLK$/MSFC57           1    004010 004177       0    040416 040420
NBSBL$/FOR              1    004200 004235
NUPDA$/FOR              1    004236 004271
NBFOO$/FOR                                       2    040421 042622
CYMODV/SC4020           1    004272 004317       0    042623 042631
                                                 2    BLANK$COMMON
CACCBY/SC4020           1    004320 004341       0    042632 042642
                                                 2    BLANK$COMMON
CXMODV/SC4020           1    004342 004367       0    042643 042651
                                                 2    BLANK$COMMON
CONCAT/MSFC             1    004370 004541       0    042652 042673
SETINT/SC4020           1    004542 004574       0    042674 042701
                                                 2    BLANK$COMMON
CHOLLV/SC4020           1    004575 004657       0    042702 042716
                                                 2    BLANK$COMMON
```

CNONLN/SC4020	1	004660 005265	0	042717 042770
			2	BLANK$COMMON
CLINRV/SC4020	1	005266 006127	0	042771 043070
	3	GGG	2	BLANK$COMMON
CYSCLV/SC4020	1	006130 006332	0	043071 043117
	3	GGG	2	BLANK$COMMON
CXSCLV/SC4020	1	006333 006535	0	043120 043146
	3	GGG	2	BLANK$COMMON
CERNLV/SC4020	1	006536 006712	0	043147 043161
			2	BLANK$COMMON
CERRLN/SC4020	1	006713 007022	0	043162 043177
			2	BLANK$COMMON
CSETCV/SC4020	1	007023 007063	0	043200 043210
			2	BLANK$COMMON
NEXP5$/FOR57	1	007064 007147	2	043211 043220
CSETMV/SC4020	1	007150 007226	0	043221 043235
			2	BLANK$COMMON
CFRAM/SC4020	1	007227 007446	0	043236 043322
	3	GGG	2	BLANK$COMMON
CXAXIS/SC4020	1	007447 007652	0	043323 043356
			2	BLANK$COMMON
VCHARV/SC4020	1	007653 010116	0	043357 043376
RITE2V/SC4020	1	010117 010347	0	043377 043425
BPLOTK/SC4020	1	010350 010430	0	043426 044005
			2	BLANK$COMMON
CCAMRA/SC4020	1	010431 010502	0	044006 044017
	3	GGG	2	BLANK$COMMON
TABLIV/SC4020			0	044020 044340
NBDCV$/FOR57	1	010503 010636	2	044341 044400
NCNVT$/FOR57	1	010637 011071	2	044401 044470
NOTIN$/MSFC55	1	011072 011422	2	044471 044501
NOUT$/FOR57	1	011423 012377	2	044502 044532
NIOER$/MSFC57	1	012400 012557	2	044533 044655
NININ$/MSFC55	1	012560 013011	2	044656 044677
NINPT$/FOR57	1	013012 013671	2	044700 044722
NFMT$/FOR57	1	013672 014576	2	044723 044741
NFCHK$/MSFC57	1	014577 015415	2	044742 045116
			4	045117 045170
NTAB$/MSFC55			2	045171 045257
CPLOTV/SC4020	1	015416 015567	0	045260 045317
	3	GGG	2	BLANK$COMMON
CLINEV/SC4020	1	015570 016153	0	045320 045376
			2	BLANK$COMMON
YSCLVI/SC4020	1	016154 016272	0	045377 045407
	3	GGG	2	BLANK$COMMON
XSCLVI/SC4020	1	016273 016410	0	045410 045420
	3	GGG	2	BLANK$COMMON
CAPLOT/SC4020	1	016411 016653	0	045421 045474
	3	GGG	2	BLANK$COMMON
CAPRNV/SC4020	1	016654 016736	0	045475 045513
			2	BLANK$COMMON
CPRNTV/SC4020	1	016737 017330	0	045514 045550
	3	GGG	2	BLANK$COMMON
CGRDIV/SC4020	1	017331 020235	0	045551 045664
	3	GGG	2	BLANK$COMMON
CDXDYV/SC4020	1	020236 021030	0	045665 045751

```
                                                              2   BLANK$COMMON
CBRITV/SC4020              1   021031 021132                  0   045752 045765
                           3   GGG                            2   BLANK$COMMON
CMARGN/SC4020              1   021133 021211                  0   045766 046027
                                                              2   BLANK$COMMON
CNBLNK/SC4020              1   021212 021261                  0   046030 046043
                                                              2   BLANK$COMMON
BMOV/MSFC                                                     0   046044 046120
CIDENT/SC4020              1   021262 022431                  0   046121 046304
                           3   GGG                            2   BLANK$COMMON
ERU$/MSFC55
DSQRT$/FOR57               1   022432 022501                  2   046305 046323
SQRT$/FOR55                1   022502 022541                  2   046324 046335
DEXP$/FOR54                1   022542 022710                  2   046336 046371
EXP$/FOR57                 1   022711 022777                  2   046372 046412
DLOG$/FOR54                1   023000 023120                  2   046413 046517
NLOUT$/MSFC55              1   023121 024206                  2   046520 046563
NLINP$/MSFC57              1   024207 025753                  2   046564 046775
NOBUF$/FOR51               1   025754 026013
NIER$/FOR52                1   026014 026076                  2   046776 047125
NIBUF$/FOR52               1   026077 026140
H$MONITOR/MSFC55           1   026141 027250                  2   047126 047703
NERR$/FOR57                1   027251 027605                  2   047704 050060
GGG (COMMON BLOCK)                                                050061 050214
CQUIKL/SC4020              1   027606 030217                  0   050215 050277
                           3   GGG                            2   BLANK$COMMON
IDENT/SC4020               1   030220 031154                  0   050300 051772
TRACE                      1   031155 031300                  0   051773 052000
                                                              2   052001 052063
INVRT                      1   031301 031713                  0   052064 052227
                                                              2   BLANK$COMMON
BLANK$COMMON (COMMON BLOCK)
LQCEXP                     1   031714 037532                  0   052230 076226
                                                              2   BLANK$COMMON


SYS$*RLIB$. LEVEL M57-0
END OF COLLECTION - TIME 3.972 SECONDS
```

@XQT EXPO

Typical Output Results for Set 1
Data Using a Two-Term Exponential Model

```
$INPUT
 T        =         .000000000000000000D+000,         .200000000000000000D+001,
                    .400000000000000000D+001,         .599999999999999999D+001,
                    .799999999999999999D+001,         .100000000000000000D+002,
                    .120000000000000000D+002,         .140000000000000000D+002,
                    .160000000000000000D+002,         .180000000000000000D+002,
                    .200000000000000000D+002,         .220000000000000000D+002,
                    .240000000000000000D+002,         .260000000000000000D+002,
                    .280000000000000000D+002,         .300000000000000000D+002,
                    .320000000000000000D+002,         .340000000000000000D+002,
                    .360000000000000000D+002,         .380000000000000000D+002,
                    .400000000000000000D+002,         .420000000000000000D+002,
                    .439999999999999999D+002,         .460000000000000000D+002,
                    .480000000000000000D+002,         .500000000000000000D+002,
                    .520000000000000000D+002,         .539999999999999999D+002,
                    .560000000000000000D+002,         .579999999999999999D+002,
                    .599999999999999999D+002,         .619999999999999999D+002,
                    .639999999999999999D+002,         .660000000000000000D+002,
                    .679999999999999999D+002,         .700000000000000000D+002,
                    .719999999999999999D+002,         .740000000000000000D+002,
                    .759999999999999999D+002,         .780000000000000000D+002,
                    .799999999999999999D+002,         .820000000000000000D+002,
                    .839999999999999999D+002,         .860000000000000000D+002,
                    .879999999999999999D+002,         .900000000000000000D+002,
                    .919999999999999999D+002,         .940000000000000000D+002,
                    .959999999999999999D+002,         .980000000000000000D+002,
                    .100000000000000000D+003,         .102000000000000000D+003,
                    .104000000000000000D+003,         .106000000000000000D+003,
                    .108000000000000000D+003,         .110000000000000000D+003,
                    .112000000000000000D+003,         .114000000000000000D+003,
                    .116000000000000000D+003,         .118000000000000000D+003,
                    .120000000000000000D+003,         .122000000000000000D+003,
                    .124000000000000000D+003,         .126000000000000000D+003,
                    .128000000000000000D+003,         .130000000000000000D+003,
                    .132000000000000000D+003,         .134000000000000000D+003,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000,
                    .000000000000000000D+000,         .000000000000000000D+000
          =         .130000000000000000D+001,         .740000000000000000D+000,
                    .613000000000000000D+000,         .530000000000000000D+000,
                    .470000000000000000D+000,         .425000000000000000D+000,
                    .385000000000000000D+000,         .345000000000000000D+000,
```

```
.3100000000000000000D+000,          .2800000000000000000D+000,
.2550000000000000000D+000,          .2300000000000000000D+000,
.2100000000000000000D+000,          .1950000000000000000D+000,
.1850000000000000000D+000,          .1750000000000000000D+000,
.1650000000000000000D+000,          .1550000000000000000D+000,
.1500000000000000000D+000,          .1450000000000000000D+000,
.1400000000000000000D+000,          .1350000000000000000D+000,
.1300000000000000000D+000,          .1250000000000000000D+000,
.1250000000000000000D+000,          .1200000000000000000D+000,
.1200000000000000000D+000,          .1150000000000000000D+000,
.1150000000000000000D+000,          .1100000000000000000D+000,
.1100000000000000000D+000,          .1050000000000000000D+000,
.1050000000000000000D+000,          .1050000000000000000D+000,
.1000000000000000000D+000,          .1000000000000000000D+000,
.1000000000000000000D+000,          .1000000000000000000D+000,
.9499999999999999999D-001,          .9499999999999999999D-001,
.9499999999999999999D-001,          .8999999999999999999D-001,
.8999999999999999999D-001,          .8999999999999999999D-001,
.8499999999999999999D-001,          .8499999999999999999D-001,
.8499999999999999999D-001,          .8499999999999999999D-001,
.8499999999999999999D-001,          .8499999999999999999D-001,
.7999999999999999999D-001,          .7999999999999999999D-001,
.7999999999999999999D-001,          .7999999999999999999D-001,
.7999999999999999999D-001,          .7999999999999999999D-001,
.7999999999999999999D-001,          .7999999999999999999D-001,
.7999999999999999999D-001,          .7999999999999999999D-001,
.7999999999999999999D-001,          .7499999999999999999D-001,
.7499999999999999999D-001,          .7499999999999999999D-001,
.7499999999999999999D-001,          .7499999999999999999D-001,
.7499999999999999999D-001,          .7499999999999999999D-001,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000,
.0000000000000000000D+000,          .0000000000000000000D+000
NN       =           +68
TL       =    .00000000E+00
TR       =    .15000000E+03
YB       =    .00000000E+00
YT       =    .20000000E+01
YB1      =   -.10000000E+01
YT1      =    .10000000E+01
VARY     =    .10000000E+01
TOLER    =    .10000000E+05
ITERM4   =             +0
```

```
ITERM3  =            +1
ITERM2  =            +0
$END
```

INITIAL ESTIMATES FOR TWO-TERM EXPONENTIAL MODEL

I	F	A1	B1	A2	B2
1	.590963+01	.215863+01	.801143-01	.750000-01	-.148030-15
2	.196719+01	.152464+01	.718354-01	.750000-01	.000000
3	.500553+00	.104223+01	.626321-01	.750000-01	.000000
4	.339488+00	.687734+00	.524097-01	.750000-01	.000000
5	.751035+00	.436815+00	.410624-01	.750000-01	-.362522-16
6	.177415+01	.143947+00	.262821-01	.106386+00	.268911-02
7	.191917+01	.100484+00	.165219-01	.122265+00	.376475-02
8	.190504+01	.978026-01	.147689-01	.127769+00	.410700-02
9	.186429+01	.101178+00	.156778-01	.127769+00	.410700-02
10	.192071+01	.971186-01	.173734-01	.125225+00	.394904-02
11	.181897+01	.118473+00	.211404-01	.121696+00	.372338-02
12	.174347+01	.136673+00	.250453-01	.117949+00	.347515-02
13	.166707+01	.156334+00	.294937-01	.114336+00	.322693-02
14	.152889+01	.189219+00	.342206-01	.111003+00	.298965-02
15	.137230+01	.228518+00	.390007-01	.107997+00	.276820-02
16	.122094+01	.272315+00	.459700-01	.105314+00	.256422-02
17	.128961+01	.248492+00	.424049-01	.109156+00	.285635-02
18	.129204+01	.244959+00	.420009-01	.111471+00	.302838-02
19	.126053+01	.251692+00	.429768-01	.112668+00	.311640-02
20	.120205+01	.266993+00	.451249-01	.113065+00	.314554-02
21	.111543+01	.291385+00	.480171-01	.112902+00	.313353-02
22	.100508+01	.324914+00	.515887-01	.112356+00	.309294-02
23	.105643+01	.310743+00	.541731-01	.115105+00	.329661-02
24	.100863+01	.319902+00	.527675-01	.116911+00	.342858-02
25	.958134+00	.335119+00	.548990-01	.117980+00	.350610-02
26	.989749+00	.322318+00	.548993-01	.121272+00	.374201-02
27	.980938+00	.322770+00	.555774-01	.123609+00	.390656-02
28	.969877+00	.328668+00	.597746-01	.125166+00	.401511-02
29	.930089+00	.333333+00	.569731-01	.128359+00	.423481-02
30	.908869+00	.338491+00	.584712-01	.130677+00	.439175-02
31	.849165+00	.356912+00	.602814-01	.132265+00	.449834-02
32	.779104+00	.382289+00	.637355-01	.133255+00	.456452-02
33	.750235+00	.392667+00	.666284-01	.135511+00	.471442-02
34	.683900+00	.417103+00	.689071-01	.137105+00	.481945-02
35	.605232+00	.451429+00	.732927-01	.138145+00	.488777-02
36	.555520+00	.477088+00	.792927-01	.140173+00	.502024-02
37	.478854+00	.512865+00	.814716-01	.141618+00	.511405-02
38	.428466+00	.540754+00	.857185-01	.143836+00	.525707-02
39	.349652+00	.592374+00	.927223-01	.145473+00	.536184-02
40	.304460+00	.621841+00	.952586-01	.147729+00	.550522-02
41	.228019+00	.690254+00	.103980+00	.149422+00	.561205-02
42	.184256+00	.734845+00	.107960+00	.151620+00	.574981-02
43	.133032+00	.809925+00	.115381+00	.153282+00	.585332-02
44	.953342-01	.921104+00	.127343+00	.155362+00	.598209-02
45	.928580-01	.929952+00	.126726+00	.157760+00	.612939-02
46	.905191-01	.975847+00	.131825+00	.160397+00	.628977-02
47	.106840+00	.107050+01	.142246+00	.163206+00	.645887-02
48	.159916+00	.118219+01	.153529+00	.166133+00	.663315-02
49	.140773+00	.115206+01	.152772+00	.169134+00	.680981-02
50	.156104+00	.118221+01	.158558+00	.172752+00	.702008-02

51	.897793-01	.102191+01	.145858+00	.176847+00	.725439-02
52	.827253-01	.951721+00	.140500+00	.181307+00	.750509-02
53	.881064-01	.886495+00	.134412+00	.186036+00	.776607-02
54	.980894-01	.840049+00	.130080+00	.191381+00	.805513-02
55	.106007+00	.810961+00	.128233+00	.197582+00	.838273-02
56	.108451+00	.797879+00	.129563+00	.204789+00	.875336-02
57	.108707+00	.790074+00	.132336+00	.212778+00	.915198-02
58	.105861+00	.789423+00	.137549+00	.221650+00	.958047-02
59	.995807-01	.798078+00	.146680+00	.231457+00	.100378-01
60	.906543-01	.819589+00	.162410+00	.242216+00	.105212-01
61	.838456-01	.850950+00	.185905+00	.253707+00	.110178-01
62	.840578-01	.890918+00	.220787+00	.265941+00	.115260-01
63	.100611+00	.944801+00	.281730+00	.279245+00	.120566-01

THE INITIAL ESTIMATES USED ARE

I= 52

NON-LINEAR EXPONENTIAL REGRESSION ANALYSIS USING AN ITERATIVE CORRECTION PROCEDURE

ASSUMED MODEL IS TWO EXPONENTIALS

INITIAL ESTIMATES FOR PARAMETERS

A1= .951721+00 B1= .140500+00 A2= .181307+00 B2= .750509-02

OBSERVED RESPONSE, COMPUTED RESPONSE, AND RESIDUALS USING INITIAL ESTIMATES

OBSERVED	COMPUTED	RESIDUAL
.130000+01	.113303+01	.166972+00
.740000+00	.897182+00	-.157182+00
.610000+00	.718490+00	-.108490+00
.530000+00	.582961+00	-.529608-01
.470000+00	.480029+00	-.100290-01
.425000+00	.401719+00	.232815-01
.385000+00	.342007+00	.429933-01
.345000+00	.296346+00	.486540-01
.310000+00	.261303+00	.486970-01
.280000+00	.234285+00	.457150-01
.255000+00	.213335+00	.416654-01
.230000+00	.196973+00	.330265-01
.210000+00	.184086+00	.259145-01
.195000+00	.173828+00	.211721-01
.185000+00	.165564+00	.194359-01
.175000+00	.158813+00	.161866-01
.165000+00	.153213+00	.117873-01
.155000+00	.148488+00	.651209-02
.150000+00	.144432+00	.556824-02
.145000+00	.140888+00	.411223-02
.140000+00	.137738+00	.226237-02
.135000+00	.134892+00	.108072-03
.130000+00	.132283+00	-.228305-02
.125000+00	.129860+00	-.485984-02
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.120000+00	.125425+00	-.542489-02
.120000+00	.123362+00	-.336156-02
.115000+00	.121377+00	-.637667-02
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.110000+00	.117594+00	-.759387-02
.110000+00	.115779+00	-.577866-02
.105000+00	.114006+00	-.900600-02
.105000+00	.112271+00	-.727145-02
.105000+00	.110572+00	-.557158-02
.100000+00	.108904+00	-.890371-02
.100000+00	.107266+00	-.726572-02
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.100000+00	.104073+00	-.407302-02
.950000-01	.102516+00	-.751584-02
.950000-01	.100984+00	-.598351-02
.950000-01	.994752-01	-.447524-02
.900000-01	.979904-01	-.799037-02
.900000-01	.965283-01	-.652833-02

.900000-01	.950886-01	-.508860-02
.850000-01	.936707-01	-.867072-02
.850000-01	.922743-01	-.727427-02
.850000-01	.908989-01	-.589886-02
.850000-01	.895441-01	-.454411-02
.850000-01	.882097-01	-.320967-02
.850000-01	.868952-01	-.189521-02
.800000-01	.856004-01	-.560041-02
.800000-01	.843250-01	-.432495-02
.800000-01	.830685-01	-.306854-02
.800000-01	.818309-01	-.183088-02
.800000-01	.806117-01	-.611679-03
.800000-01	.794107-01	.589337-03
.800000-01	.782276-01	.177245-02
.800000-01	.770621-01	.293792-02
.800000-01	.759140-01	.408602-02
.800000-01	.747830-01	.521701-02
.800000-01	.736688-01	.633115-02
.750000-01	.725713-01	.242869-02
.750000-01	.714901-01	.350987-02
.750000-01	.704251-01	.457494-02
.750000-01	.693759-01	.562414-02
.750000-01	.683423-01	.665771-02
.750000-01	.673241-01	.767589-02
.750000-01	.663211-01	.867889-02

SIGYIN= .359525-01

CYCLE NUMBER = 1

B MATRIX

.100000+01	.000000	.100000+01	.000000
.755028+00	-.143715+01	.985102+00	-.357211+00
.570068+00	-.217018+01	.970426+00	-.703779+00
.430417+00	-.245782+01	.955968+00	-.103994+01
.324977+00	-.247430+01	.941726+00	-.136593+01
.245367+00	-.233521+01	.927696+00	-.168198+01
.185259+00	-.211578+01	.913875+00	-.198830+01
.139876+00	-.186372+01	.900260+00	-.228513+01
.105610+00	-.160818+01	.886848+00	-.257266+01
.797386-01	-.136600+01	.873636+00	-.285113+01
.602049-01	-.114597+01	.860620+00	-.312073+01
.454564-01	-.951761+00	.847799+00	-.338166+01
.343209-01	-.783934+00	.835168+00	-.363412+01
.259132-01	-.641217+00	.822726+00	-.387831+01
.195652-01	-.521378+00	.810469+00	-.411442+01
.147723-01	-.421773+00	.798394+00	-.434263+01
.111535-01	-.339681+00	.786500+00	-.456313+01
.842121-02	-.272498+00	.774782+00	-.477609+01
.635825-02	-.217846+00	.763240+00	-.498170+01
.480066-02	-.173618+00	.751869+00	-.518012+01
.362463-02	-.137986+00	.740667+00	-.537152+01
.273670-02	-.109392+00	.729633+00	-.555607+01
.206629-02	-.865273-01	.718763+00	-.573393+01
.156010-02	-.683001-01	.708055+00	-.590525+01
.117792-02	-.538106-01	.697506+00	-.607020+01

.889365-03	-.423214-01	.687114+00	-.622892+01
.671496-03	-.332320-01	.676878+00	-.638157+01
.506998-03	-.260561-01	.666794+00	-.652828+01
.382798-03	-.204018-01	.656860+00	-.666921+01
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.124401-03	-.757726-02	.618582+00	-.717780+01
.939260-04	-.589983-02	.609366+00	-.729182+01
.709168-04	-.458952-02	.600288+00	-.740086+01
.535442-04	-.356714-02	.591345+00	-.750503+01
.404274-04	-.277024-02	.582535+00	-.760446+01
.305238-04	-.214971-02	.573856+00	-.769925+01
.230463-04	-.166696-02	.565307+00	-.778954+01
.174006-04	-.129172-02	.556885+00	-.787542+01
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.991954-05	-.774132-03	.540415+00	-.803444+01
.748953-05	-.598748-03	.532364+00	-.810778+01
.565481-05	-.462835-03	.524433+00	-.817716+01
.426954-05	-.357580-03	.516620+00	-.824267+01
.322362-05	-.276119-03	.508923+00	-.830441+01
.243393-05	-.213111-03	.501341+00	-.836248+01
.183768-05	-.164402-03	.493872+00	-.841698+01
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.597205-06	-.579740-04	.465092+00	-.860109+01
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.257047-06	-.264208-04	.444614+00	-.870603+01
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.146534-06	-.156195-04	.431464+00	-.876147+01
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.835345-07	-.922218-05	.418704+00	-.880601+01
.630709-07	-.708306-05	.412466+00	-.882439+01
.476203-07	-.543855-05	.406321+00	-.884026+01
.359547-07	-.417470-05	.400268+00	-.885370+01
.271468-07	-.320369-05	.394305+00	-.886477+01
.204966-07	-.245789-05	.388430+00	-.887356+01
.154755-07	-.188523-05	.382643+00	-.888011+01
.116844-07	-.144564-05	.376943+00	-.888450+01
.882209-08	-.110829-05	.371327+00	-.888678+01
.666093-08	-.849473-06	.365795+00	-.888703+01

BT*W*B

.232595+01	-.587038+01	.390289+01	-.410829+01
-.587038+01	.408060+02	-.215654+02	.532206+02
.390289+01	-.215654+02	.294226+02	-.241823+03
-.410829+01	.532206+02	-.241823+03	.321212+04

INVERSE OF BT*W*B

.856977+00	.121971-01	-.255456+00	-.183380-01
.121971-01	.805688-01	.122212+00	.788133-02
-.255456+00	.122212+00	.362295+00	.249237-01
-.183380-01	.788133-02	.249237-01	.203365-02

INVERSE TIMES ORIGINAL MATRIX

.100000+01	-.607153-17	.693889-17	-.555112-16
.271051-18	.100000+01	-.173472-17	.277556-16

.000000	.693889-17	.100000+01	.000000
.135525-18	-.650521-18	.433681-18	.100000+01

DETERMINANT VALUE

.522963+06

OBSERVED RESPONSE, COMPUTED RESPONSE AND RESIDUALS

OBSERVED	COMPUTED	RESIDUAL
.130000+01	.115504+01	.144964+00
.740000+00	.895831+00	-.155831+00
.610000+00	.706661+00	-.966608-01
.530000+00	.568294+00	-.382939-01
.470000+00	.466786+00	.321428-02
.425000+00	.392026+00	.329741-01
.385000+00	.336684+00	.483163-01
.345000+00	.295444+00	.495561-01
.310000+00	.264452+00	.455478-01
.280000+00	.240914+00	.390862-01
.255000+00	.222802+00	.321982-01
.230000+00	.208646+00	.213536-01
.210000+00	.197381+00	.126187-01
.195000+00	.188233+00	.676698-02
.185000+00	.180640+00	.435966-02
.175000+00	.174196+00	.804076-03
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.100000+00	.110848+00	-.108476-01
.100000+00	.108485+00	-.848530-02
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.950000-01	.101701+00	-.670129-02
.950000-01	.995366-01	-.453659-02
.950000-01	.974183-01	-.241825-02
.900000-01	.953452-01	-.534522-02
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.850000-01	.893878-01	-.438779-02
.850000-01	.874860-01	-.248603-02
.850000-01	.856248-01	-.624774-03
.850000-01	.838031-01	.119686-02
.850000-01	.820203-01	.297971-02
.850000-01	.802754-01	.472461-02

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.800000-01     .785676-01     .143239-02
.800000-01     .768962-01     .310382-02
.800000-01     .752603-01     .473969-02
.800000-01     .736592-01     .634076-02
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.800000-01     .661506-01     .138494-01
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.750000-01     .606987-01     .143013-01
.750000-01     .594074-01     .155926-01
.750000-01     .581436-01     .168564-01
.750000-01     .569067-01     .180933-01
.750000-01     .556961-01     .193039-01
.750000-01     .545112-01     .204888-01


 PARAMETER CORRECTIONS
DELA1=  -.269235-01   DELB1=   .202625-01   DELA2=   .489308-01   DELB2=   .324644-02


 IMPROVED PARAMETER ESTIMATES
A1=   .924798+00   B1=   .160783+00   A2=   .230238+00   B2=   .107515-01


 RESPONSE VARIABLE STANDARD DEVIATION
SIGY1=   .359525-01   SIGY2=   .341503-01


 COEFFICIENT STANDARD DEVIATION
SGA1=   .223921-01   SGB1=   .534604-02   SGA2=   .629584-02   SGB2=   .602557-03


 TOLER=  -.126342-03
END OF CYCLE NUMBER   1
```

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APPROVAL

A METHOD FOR NONLINEAR EXPONENTIAL REGRESSION ANALYSIS

By Bobby G. Junkin

The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

H. Hoelzer

H. HOELZER
Director, Computation Laboratory

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