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GREEN, Jr., Ernest Jackson, 1934-
THE STEP RESPONSE ANALYSIS OF A CHEMICAL REACTOR SYSTEM WITH MEASUREMENT ERROR.

Rice University, Ph.D., 1965
Engineering, chemical

University Microfilms, Inc., Ann Arbor, Michigan
RICE UNIVERSITY

THE STEP RESPONSE ANALYSIS
OF A CHEMICAL REACTOR SYSTEM
WITH MEASUREMENT ERROR

by

ERNEST J. GREEN, JR.

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY IN CHEMICAL ENGINEERING

Thesis Director's signature

Houston, Texas
June, 1964
ACKNOWLEDGMENTS

The author would like to express his sincere appreciation to the following organizations and persons:

Dr. Sam H. Davis - for his guidance and assistance in this problem,

The Rice University Computer Project - for the use of the computer facilities and the aid of the programming staff,

Rice University - for financial support,

My wife, sons, and our parents - for support, faith, and inspiration.
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NOMENCLATURE

Roman Letters:

A  Amplitude of step disturbance = $\bar{T} - \bar{T}_0$
A  Constant 4 x 4 matrix
a  Real part of complex root in step response expression
aij  Elements of matrix in Appendix B
A,B,C,D,E,F  Chemical species
aj  Decay factor in step response expression
a  Vector in Appendix B
B  Constant 4 x 4 matrix
b  Imaginary part of complex root in step response expression
C  Constant 4 x 2 matrix
C  Constant 4 x 4 matrix in Appendix A
c  Vector of coefficients in step response expression
C_{ij}  Coefficient in step response expression
C_p  Molal specific heat
D  Fractional root mean square deviation of non-linear system response from linearized system response to a step disturbance
D  Constant 4 x 2 matrix in Appendix A
D_1  Value of determinant in Appendix B
E  Constant 4 x 2 matrix in Appendix A
$\Delta E_1$  Activational energy
F  Range of measurement error, $-F \leq 0 \leq F$
F_1  Molal feed rate
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\[ r \] Vector of reaction rate deviations

\[ r_{ij} \] First order term in Taylor series expansion of reaction rate expression, \( \partial r_i / \partial x_j \)

\[ r_i \] Decay factor in Prony method step response expression \( r_i = a_i \Delta t \)

\[ s \] Laplace transform variable

\[ t \] Time

\[ T \] Absolute temperature

\[ T_c \] Coolant temperature

\[ T' \] Environment temperature

\[ \Delta t \] Time spacing between discrete observations of system response

\[ T \] Total observation time, \( T = N \Delta t \)

\[ U \] Heat transfer coefficient

\[ x_i \] Specie mol fraction

\[ x \] Time variable in Prony method \( x = t / \Delta t \)

\[ x \] Step response vector in Appendix A

\[ Y \] \((N-3) \times 4\) matrix in Appendix B

\[ y \] Vector of reactor state deviations

\[ y' \] Observed value of step response

\[ y_i \] Reactor state deviation

\[ z \] Vector of feed state deviations

\[ z_i \] Feed state deviation

Greek Letters:

\[ \lambda \] Parameter in definition of random function
\( \alpha_i, \beta, \gamma_i \) Intermediate parameters in Prony method

\( \beta \) Heat flow and transfer coefficient = \( 1 + \frac{U}{Re \, C_p} \)

\( \gamma_i \) Reaction rate heat release = \(-H_i/C_p\)

\( \varepsilon \) Error in observing step response, Appendix B

\( \xi \) Convergence criterion of numerical solution

\( \eta \) Vector in Appendix B

\( \Theta \) Imaginary part of complex root in Prony method, \( \Theta = b \Delta t \)

\( \mathcal{H}_i \) Transformed counterpart of exponential in Prony method, \( \mathcal{H}_1 = e^{\mathcal{R}_1} \)

\( \xi \) Vector in Appendix B

\( \tau \) Time variable

\( \tau \) Time variable

\( \Phi_{11}(t) \) Autocorrelation function of random signal

\( \Phi_{11}(s) \) Spectral density function of random signal

\( \varphi \) Mean square value of response of linear system to random signal defined by \( \Phi_{11}(s) \)

\( \varphi_1 \) Mean square value of response of fitted linear system to random signal defined by \( \Phi_{11}(s) \)

\( \varphi_e \) Error criterion for measuring success of step response analysis, \( \varphi_e = 10^5 (\varphi_1 - \varphi) \)

\( \overline{\varphi^2} \) Average value of error criterion

\( \overline{\varphi^2} \) Mean square value of error criterion

Subscripts:

A,B,C Component designation indices

c Coolant

F Feed stream

I Imaginary part of complex root

i,j,k General indices
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<td>m</td>
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I. Introduction

Two factors which complicate the transient response analysis of a chemical reactor system are (1) the non-linear character of the chemical system and (2) measurement errors made in observing the system.

A large number of techniques have been proposed for the transient analysis of linear systems. These consist mainly of disturbing the system from some steady state condition, observing the system response to the disturbance, and fitting the observed response to a model describing the system. Examples of several of these are presented by Del Toro and Parker\textsuperscript{4} and by Mishkin and Braun\textsuperscript{9}. It has been shown that under certain conditions chemical reactor systems approach linear behavior\textsuperscript{3, 7}. It has further been shown that under these conditions several of the linear transient response techniques give satisfactory results in analyzing chemical systems\textsuperscript{1, 6}.

The assumption of linear behavior is usually justified by defining the system variables as deviations from a steady state condition with the restraint that the magnitudes of the deviations are small. Thus in the transient analysis of a chemical system subject to these conditions, the amplitude of the disturbance must be small. The opposite is true, however, for linear systems analyzed in the presence of measurement error. To reduce the effects of measurement
error on the transient analysis of the linear system, the amplitude of the disturbance is increased. The transient response analysis of a chemical reactor system must compromise between these two conflicting requirements when measurement error is present. It is thus necessary to know how system non-linearity and measurement error combine to affect the transient analysis.

The purpose of this paper is to study the effects of system non-linearity and measurement error on the transient response analysis of a chemical reactor system. This is done by digital computer simulation of the step response analysis of a continuous stirred tank chemical reactor. The dynamic behavior of a stirred tank chemical reactor can be described by the set of non-linear differential equations of the form:

\[
\frac{dy}{dt} = f(y) + Pz
\]  

(1)

based on material and energy balances about the system. Numerical solution of this set of non-linear equations for a step disturbance in z yields the response of the non-linear system which is to be analyzed.

Linearization of this set of equations for small magnitude disturbances about a steady state condition gives the set of linear equations:

\[
\frac{dy}{dt} + Fy = Pz
\]  

(2)
The analytical solution of this set of linear equations for a step disturbance in $z$ is used as the response of the linear system which is to be compared in various ways to the observed behavior of the non-linear system. The solution of the response of any variable $y_1$ to a step in $z_k$ is of the form

$$y_1^k(t) = c_{10}^k + \sum_{j=1}^{n} c_{ij}^k e^{ajt} \quad (3)$$

In the transient analysis of a system using a digital computer, discrete observations of the response of the system to some disturbance are used to evaluate parameters in a model describing the system. The form of the model used depends to a large extent on the system complexity and the availability of a theoretical description of the system. In this analysis it is assumed that the form of the set of non-linear differential equations describing the stirred tank chemical reactor is known but that values of the parameters, i.e. heats of reaction, reaction rates, heat transfer coefficients, etc., are unknown. The model used to fit the discrete observations of the response of the non-linear system and the linear system to a step in $z$ has the form of Equation (3), the analytical solution of the step response of the linear system. This provides a convenient comparison of the fitted model to the linearized system. A measure of the goodness of the fit will be defined based on this comparison.
Before performing the transient analysis of a system, values of parameters necessary in the execution of the method of analysis must be chosen. In the step response analysis these are:

1. $\Delta t$, the time spacing between discrete observations of the system response
2. $N$, the number of observations
3. $A$, the amplitude of the step disturbance.

One of the objects of this paper is to determine whether some combination of these parameters minimizes the combined effect of system non-linearity and measurement error. The investigation of the relationships between these parameters, system non-linearity, and measurement error consists of simulating the analysis of the following systems:

1. Non-linear and linear systems without measurement error
2. Linear system with measurement error
3. Non-linear system with measurement error.

This procedure simplifies the comparison of the contribution of the individual effects with the combined contribution of system non-linearity and measurement error. The results of this, as well as the relationships with the parameters $\Delta t$, $N$, and $A$ are discussed in detail in the following sections.
II. Theory

The purpose of this section is to develop the equations used to simulate the step response analysis of the stirred tank chemical reactor. The set of non-linear differential equations that describes the transient response of the stirred tank chemical reactor is derived. Subsequent linearization of this set of equations gives the set of linear equations that approximates the behavior of the system for small disturbances about a steady state. The analytical solution of this linear system for a step disturbance provides the form of the model used to fit the observed values of the response of both the non-linear and linear systems to step disturbances. Finally, the method used to fit the observed response to the model is presented.

The continuous stirred tank chemical reactor system used in this analysis is the same as that used by Davis\(^3\). The behavior of the reactor is dominated by two second order irreversible reactions:

\[ \text{A + B} \rightarrow \text{C + D} \quad (4) \]
\[ \text{A + C} \rightarrow \text{E + F} \quad (5) \]

The following assumptions and conditions define the reactor system:

(1) The feed to the reactor is a mixture of A and B.
(2) The molal feed and product rates are constant, with resulting constant molal hold up in the reactor.
(3) Energy losses are approximately given by
\[ q = U(T - T_c) \] with constant U.

(4) The reaction rates are given by Arrhenius relations
for second order reactions:
\[ r_1 = k_1 x_A x_B \exp\left(-\frac{\Delta E_1}{RT}\right) \] (6)
\[ r_2 = k_2 x_A x_C \exp\left(-\frac{\Delta E_2}{RT}\right). \] (7)

(5) The reactor is stirred so that the composition
and temperature of its contents are constant
throughout and these are the composition and
temperature of the product stream.

With these assumptions, a set of state variables for
the reactor are \((x_A, x_B, x_C, T)\) with the feed condition at
any instant given by \((x_{A_F}, T_F)\). The equations which describe
the transient behavior of the reactor may be written as:

\[ \frac{dx_A}{dt} = x_{A_F} - x_A - r_1 - r_2 \] (8)

\[ \frac{dx_B}{dt} = 1 - x_{A_F} - x_B - r_1 \] (9)

\[ \frac{dx_C}{dt} = -x_C + r_1 - r_2 \] (10)

\[ \frac{dT}{dt} = (T - T) + \gamma_1 r_1 + \gamma_2 r_2 \] (11)

with time, \(t\), given in reactor throughputs. The temperature,
\(T\), is a function of the feed and coolant temperatures
given by:
\[ T = \frac{T_F + (\beta - 1)T_C}{\beta} \]  
(12)

Other groups appearing in the equations are the heat flow and transfer coefficient:
\[ \beta = 1 + \frac{U}{Rc_p} \]  
(13)

and the reaction rate heat release:
\[ \gamma_i = \frac{-H_i}{C_p} \quad i = 1, 2. \]  
(14)

Since the step response analysis depends on linear behavior of the system analyzed, it must be conducted so that the chemical reactor system approaches linear behavior. This is done by applying the step disturbance so that the system response occurs as small deviations from a steady state condition. It is convenient then to define the state variables of the chemical reactor system in terms of deviations of the reactor state and feed state from steady state condition. A steady state reference vector \((x_{A_0}, x_{B_0}, x_{C_0}, \quad T_0)\) is defined as the solution of Equations (8, 9, 10, and 11) for the conditions:
\[ \left(\frac{dx_A}{dt}\right)_0 = \left(\frac{dx_B}{dt}\right)_0 = \left(\frac{dx_C}{dt}\right)_0 = \left(\frac{dT}{dt}\right)_0 = 0 \]  
(15)
and the solution of the equations resulting from the requirements:

$$\left( \frac{\partial x_C}{\partial x_{A_F}} \right) = 0$$  \hspace{1cm} (16)

and

$$\left( \frac{\partial x_C}{\partial T} \right) = 0$$  \hspace{1cm} (17)

Solution of the six resulting algebraic equations for

$$(x_{A_{F_o}}, T_o, x_{A_o}, x_{B_o}, x_{C_o}, T_o)$$

for any given system parameters ($\beta$, $\gamma_1$, $\gamma_2$, $k_1$, $k_2$, $\Delta E_1$, $\Delta E_2$) gives the steady state operating point for optimum yields of $x_C$. This will be used as the basis of the steady state condition.

The state variables defining the stirred tank reactor can now be defined as:

$$y \equiv (x_A - x_{A_o}, x_B - x_{B_o}, x_C - x_{C_o}, T - T_o)$$  \hspace{1cm} (18)

and

$$z \equiv (x_{A_{F_o}} - x_{A_o}, T - T_o)$$  \hspace{1cm} (19)

where $y$ and $z$ are written as deviations from a steady state condition. The set of differential equations then becomes:

$$\frac{dy_1}{dt} = z_1 - y_1 - R_1 - R_2$$  \hspace{1cm} (20)

$$\frac{dy_2}{dt} = -z_1 - y_2 - R_1$$  \hspace{1cm} (21)

$$\frac{dy_3}{dt} = -y_3 \ast R_1 - R_2$$  \hspace{1cm} (22)
\[
\frac{d\gamma_4}{dt} = \beta (z_2 - \gamma_4) + \chi_1 R_1 + \chi_2 R_2
\] (23)

where \( R_1 = r_1 - r_1^0 \), \( R_2 = r_2 - r_2^0 \). A compact representation of these equations is:

\[
\frac{d\gamma}{dt} = My + Nr + Pz
\] (24)

where \( M \) is a constant \( 4 \times 4 \) matrix, \( N \) and \( P \) are constant \( 4 \times 2 \) matrices,

and

\[
\gamma = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}.
\] (25)

Pre-multiplication of the terms of matrix Equation (24) by the constant matrix:

\[
A = \begin{bmatrix}
1 & -2 & -1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & \chi_1 + \chi_2 & \chi_2 & 1
\end{bmatrix}
\] (26)

minimizes the appearance of the non-linear reaction rate terms \( R_1 \) and \( R_2 \). Thus:

\[
A \frac{d\gamma}{dt} = AMy + ANr + APz
\] (27)

where

\[
AN = \begin{bmatrix}
0 & 0 \\
-1 & 0 \\
0 & -1 \\
0 & 0
\end{bmatrix}.
\] (28)
A numerical solution of the set of non-linear differential equations represented by Equation (27) provides discrete values of the step response of the non-linear system.

For small variations of the system variables about the steady state, a Taylor series expansion of the reaction rate expressions gives:

\[ R_1 = r_{11} y_1 + r_{12} y_2 + r_{14} y_4 + \cdots \]  \hspace{1cm} (29)

and

\[ R_2 = r_{21} y_1 + r_{23} y_3 + r_{24} y_4 + \cdots \]  \hspace{1cm} (30)

where

\[ r_{ij} = \frac{\partial r_i}{\partial x_j} \]  \hspace{1cm} (31)

with

\[ x_1 = x_A, \ x_2 = x_B, \ x_3 = x_C, \ x_4 = T. \]  \hspace{1cm} (32)

Substitution of the expressions for \( R_1 \) and \( R_2 \) in Equation (27) results in the linear approximation:

\[ A \frac{dy}{dt} + By = Cz \]  \hspace{1cm} (33)

where

\[ B = \begin{bmatrix} 1 & -2 & -1 & 0 \\ r_{11} & (1+r_{12}) & 0 & r_{14} \\ r_{21} & 1 & (1+r_{23}) & r_{24} \\ 0 & (\alpha_1 + \alpha_2) & \beta_{12} & 0 \end{bmatrix} \]  \hspace{1cm} (34)

An analytical solution of the response of this linear system to a step in \( z \) is possible. For the initial conditions:

\[ y_1 = y_2 = y_3 = y_4 = 0, \ t = 0 \]  \hspace{1cm} (35)
the Laplace transform of Equation (33) gives:

$$\left[ sA + B \right] y(s) = Cz(s)$$  \hspace{1cm} (36)

or

$$Qy(s) = Cz(s)$$  \hspace{1cm} (37)

Solving for $y(s)$

$$y(s) = Q^{-1}Cz(s).$$  \hspace{1cm} (38)

A step change probe will be used to predict system behavior. For the response of a particular $y_1$ to a step in $z_2$ Equation (38) becomes:

$$y_1(s) = \frac{q_1^m(s)}{sp^n(s)}$$  \hspace{1cm} (39)

where $q_1^m(s)$ and $p^n(s)$ are polynomials in $s$ of order $m$ and $n$ respectively. The denominator polynomial is a cubic, and if the roots of the polynomial are real, the expression for $y_1$ in the time domain is given by:

$$y_1(t) = C_{10} + C_{11}e^{a_1t} + C_{12}e^{a_2t} + C_{13}e^{a_3t}.$$  \hspace{1cm} (40)

Obviously for the response to be stable, these roots must be negative. If the roots of the cubic contain the complex pair $(a + ib)$, the solution in the time domain is given by:

$$y_1(t) = C_{10} + e^{at}(C_{11}\cos bt + C_{12}\sin bt) + C_{13}e^{a_3t}.$$  \hspace{1cm} (41)

Again for the response to be stable, the roots must have negative real parts.

The response of the linearized version of the stirred tank chemical reactor to a step in $z_2$ can be evaluated for discrete values of time using this analytical solution.
It was shown earlier that discrete values of the response of the non-linear version of the stirred tank chemical reactor to a step in $z_2$ are given by the numerical solution of Equation (27). To carry out the simulation of the step response analysis of the chemical reactor system, it is now desired to fit these "observed" data to a model describing the system. The model chosen for the fit has the form of the analytical solution of the step response of the line- arized system. A method for fitting these data to this model, Prony's method\textsuperscript{5} will now be presented.

The step response of either the non-linear or the linear version of the stirred tank reactor is available as $N$ values of $y_i(t)$ at the discrete values of time, $t = 0, \Delta t, 2 \Delta t, \ldots, (N-1) \Delta t$. Time is measured from the instant of application of the step disturbance. Since the method to be developed is equally applicable to $y_1$, $y_2$, $y_3$, or $y_4$, the subscript $i$ will be dropped.

A linear change of variables is imposed such that

$$x = \frac{t}{\Delta t} \quad (42)$$

and the values of $y(x)$ are known for $N$ equally spaced points at $x = 0, 1, \ldots, N-1$. The individual data points will be designated by $y_k$, $k = 0, 1, \ldots, N-1$. It is desired to determine an approximation of the form

$$y(x) = c_0 + c_1 e^{r_1 x} + c_2 e^{r_2 x} + c_3 e^{r_3 x} \quad (43)$$
in which the C's are real and the r's are either real or occur as complex pairs. An equivalent representation is

\[ y(x) = C_0 + C_1 \mu_1^x + C_2 \mu_2^x + C_3 \mu_3^x \]  

(44)

where

\[ \mu_i = e^{ri}. \]  

(45)

For Equation (44) to be an equality for the N observed points, the following set of N equations must be satisfied:

\[ C_0 + C_1 \mu_1^k + C_2 \mu_2^k + C_3 \mu_3^k = y_k, \quad k = 0, 1, \ldots, N-1. \]  

(46)

Since this set of equations is to be solved for the parameters \( C_0, C_1, C_2, C_3, \mu_1, \mu_2, \) and \( \mu_3, \) at least \( N = 7 \) observations of the step response are needed. Solution of this set of equations is complicated by the fact that the equations are non-linear in \( \mu. \) The set of equations (46) can be written:

\[ C_1^\prime \mu_1^k + C_2^\prime \mu_2^k + C_3^\prime \mu_3^k = y_k, \quad k = 0, 1, \ldots, N-2 \]  

(47)

where

\[ y_k = y_{k+1} - y_k \]  

(48)

and

\[ C_i^\prime = C_i (\mu_i - 1). \]  

(49)

Equation (47) can be compactly represented by:

\[ Mc = f \]  

(50)

where \( M \) is the \( (N-1) \times 3 \) matrix of \( \mu_i^k, \) \( c \) is the vector of coefficients, and \( f \) is the vector of \( N-1 \) values of \( \Delta y. \)
Let $\mu_1, \mu_2, \text{and } \mu_3$ be the roots of the equation:

$$\mu^3 - \lambda_1 \mu^2 - \lambda_2 \mu - \lambda_3 = 0$$  \hspace{1cm} (51)

Then, pre-multiplication of Equation (50) by the $(N-4) \times (N-1)$ matrix of the form:

$$P = \begin{bmatrix}
\lambda_3 & \lambda_2 & \lambda_1 & -1 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & \lambda_3 & \lambda_2 & \lambda_1 & -1 & \ldots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & \lambda_3 & \lambda_2 & \lambda_1 & -1 \\
0 & 0 & 0 & 0 & 0 & \ldots & 0 & \lambda_3 & \lambda_2 & \lambda_1 & -1
\end{bmatrix}$$  \hspace{1cm} (52)

gives

$$PMc = Pf.$$  \hspace{1cm} (53)

The elements of the matrix product $PM$ are all of the form:

$$\mu_1^n (\mu_1^3 - \lambda_1 \mu_1^2 - \lambda_2 \mu_1 - \lambda_3), \hspace{1cm} n = 0, 1, \ldots, N-5,$$

and since

$$\mu_1^3 - \lambda_1 \mu_1^2 - \lambda_2 \mu_1 - \lambda_3 = 0$$  \hspace{1cm} (55)

the matrix $PM$ is null.

Thus

$$Pf = 0.$$  \hspace{1cm} (56)

The elements of $Pf$ are of the form:

$$\Delta v_n - \lambda_1 \Delta v_{n-1} - \lambda_2 \Delta v_{n-2} - \lambda_3 \Delta v_{n-3} = 0.$$  \hspace{1cm} (57)

This defines the set of $N-4$ linear algebraic equations:

$$\Delta v_{n-1} \lambda_1 + \Delta v_{n-2} \lambda_2 + \Delta v_{n-3} \lambda_3 = \Delta v_n$$  \hspace{1cm} (58)
for \( n = 3, 4, \ldots, N-2 \). Since the values of \( \Delta y_k \) are known, these equations can be solved approximately for \( N \geq 7 \) for the values of \( \alpha_1, \alpha_2, \) and \( \alpha_3 \) by least square techniques. The values of \( \mu_1, \mu_2, \) and \( \mu_3 \) are then found as the roots of Equation (51). The set of equations given by (46) are solved approximately for the coefficients \( C_0, C_1, C_2, \) and \( C_3 \) using least square techniques.

The decay factors \( r_1, r_2, \) and \( r_3 \) are determined from \( \mu_1, \mu_2, \) and \( \mu_3 \) by the relationship:

\[
    r_i = \ln \mu_i
\]  

(59)

Since the change of variables was imposed such that:

\[
    x = t / \Delta t
\]  

(60)

the following is true:

\[
    e^{r_1x} = e^{ait}
\]  

(61)

but

\[
    t = x \Delta t
\]  

(63)

so

\[
    a_i = \frac{r_i}{\Delta t}
\]  

(64)

This section has presented the relationships used in the simulation of the step response analysis of the stirred tank chemical reactor system. Methods of generating data describing the step response of both the non-linear and linear versions of the stirred tank reactor were developed, and a method for fitting these discrete data to the form of the chosen model was presented.
III. Analysis and Results

Using the methods developed in the last section, a group of programs was written to simulate the step response analysis of the stirred tank chemical reactor system on the Rice University Digital Computer. A numerical solution of the set of non-linear differential equations (17) programmed by Davis\textsuperscript{3} was used to simulate the step response of the non-linear version of the stirred tank reactor. The analytical solution of the set of linear differential equations (33) was programmed to simulate the step response of the linearized version of the system. A program was written to use the Prony method to fit the recorded response from either of these simulations to the model of the form:

$$y(t) = C_0 + C_1e^{a_1t} + C_2e^{a_2t} + C_3e^{a_3t}$$  \hspace{1cm} (65)

The transient behavior of the system to this point has only been described in terms of the step response. If the amplitude of the step disturbance is $A$, the unit impulse response of a particular variable of the system can be obtained from the fitted step response of that variable by applying the operator $\frac{1}{A} \frac{d}{dt}$. The Laplace transform of the resulting expression, of course, yields the fitted transfer function of the system.

Some error criterion for evaluating the effect of the system non-linearity and the effect of measurement error on the step response analysis must be defined. The fitted model has the form of the analytical solution of the step
response of the linear system. Thus for a given step disturbance in $z_2$ the exact values that should be taken by the parameters in the fitted model can be calculated. An obvious basis for the error criterion then is to compare the parameters in the fitted model to their exact counterpart. It is desirable for the error in a fit to be represented by the value of a single number. Thus the error criterion was defined as the sum of the absolute values of the fractional deviations of the fitted parameters ($C_0$, $C_1$, $C_2$, $C_3$, $a_1$, $a_2$, and $a_3$) from their exact values. This error criterion was found to be unsuitable due largely to the wide range of magnitudes in the parameters.

An error criterion is now defined in which the response of the fitted model is compared to the response of the linear system when they are both driven by the same signal. Define the signal $\overline{\Phi}_{11}(s)$ by its spectral density function:

$$\overline{\Phi}_{11}(s) = \frac{-1}{s^2 - 1}$$  \hspace{1cm} (66)

The mean square value of the response of the linear system is given by:

$$\varphi = e^2(t) = \frac{1}{2\pi j} \int_{-j\infty}^{j\infty} G(s) \overline{\Phi}_{11}(s)G(-s) ds$$  \hspace{1cm} (67)

where $G(s)$ is the transfer function of the linear system. A similar expression can be written for $\varphi_1$, the mean square value of the response of the fitted system, in terms of
the fitted transfer function $C_1(s)$. The error criterion is now defined as:

$$ S \phi = \left[ \phi - \phi_i \right] 10^S. \quad (68) $$

Solutions for integrals of the form of Equation (67) are tabulated in Chang. A solution for $S \phi$ was programmed in terms of the parameters of the fitted model and in terms of parameters of the linear system. This criterion will be shown to be quite suitable.

In this investigation, four versions of the stirred tank chemical reactor are used. These four versions are described by the same set of equations with different values of the system parameters. The values of the system parameters used in each version are tabulated in Table I. This tabulation also includes the roots of the characteristic equation of the linearized system, along with the steady state values of the reactor temperature, $T_0$, and the environment temperature, $\overline{T_0}$. Note that the different versions are defined such that the steady state value of the reactor temperature remains constant. The values of the activational energies, represented by $\Delta E_1$, were chosen such that the non-linear properties of Case 1 and Case 2 are accentuated. Case 3 and Case 4 are not as strongly non-linear.

The simulation of the step response analysis is limited to the response of the state variable $y_4$ to a step in $z_2$ of magnitude $A$. It was felt that this variable would most strongly reflect non-linear effects since the exponential
in temperature in the Arrhenius expression is the dominant non-linear term in the equations describing the chemical reactor system. It can be seen from the linearized system that the fitted step response of \( y_1, y_2, \) or \( y_3 \) should differ from the step response of \( y_4 \) only in the values of the C's; the a's given by the roots of the characteristic equation of the system remaining constant. As long as the property of superposition holds, this is true.

The digital computer simulation of the step response analysis of the stirred tank chemical reactor for a given set of analysis parameters (\( \Delta t, N, \) and \( A \)) proceeds in the following manner.

1. The response of \( y_4 \) to a step in \( z_2 \) of amplitude \( A \) is generated by the numerical solution of the set of non-linear equations which describes the stirred tank reactor. Precautions are taken to insure consistent accuracy in the computer program that performs the numerical integration. The time step used in the solution is kept constant at \( \Delta t_s = 0.0125 \). Thus, the time increment between observations, \( \Delta t \), must be some even multiple of 0.0125. Further, the convergence criterion in the numerical solution is set at \( \varepsilon = 10^{-9} \). The value of \( y_4 \) is recorded at a time spacing of \( \Delta t \) until \( N \) discrete values have been generated.

2. Depending on the condition of an externally set switch on the computer, these values are observed with or without measurement error. Measurement error is simulated
by generating a sequence of N random numbers with values between -1.0 and +1.0. These numbers are then multiplied by a factor F such that the range of values of the numbers is \(-F \leq 0 \leq F\). These N values are then superimposed on the N values of \(y_4\).

3. The N values of \(y_4\), with or without measurement error, are fitted to the model:

\[ y(t) = c_0 + c_1e^{a_1t} + c_2e^{a_2t} + c_3e^{a_3t} \]  

(69)

using the Prony method.

4. The true values of the parameters of the linear system are then calculated for the case being analyzed. The value of the error criterion is then calculated from these exact parameters and the fitted parameters.

5. The analytical solution of the linearized set of system equations generates N values of the response of \(y_4\) to a step in \(z_2\) of amplitude A. This response of \(y_4\) based on the linear system is generated and recorded at a time spacing of \(\Delta t\).

6. Steps 2, 3, and 4 are repeated for the response of the linearized system.

The analysis and results of this investigation will be presented in the three phases indicated in the introduction:

1. Non-linear and linear systems without measurement error,
2. Linear system with measurement error, and
3. Non-linear system with measurement error.

This procedure is intended to show how the non-linear effects observed in phase 1 combine with the measurement error effects observed in phase 2 to produce the combined effects observed in phase 3. The analysis parameters $\Delta t$, $N$, and $A$ are varied systematically in each phase to determine how the choice of these variables influences the results of the analysis. The error criterion $\delta\Psi$, as defined earlier, provides the measure of these effects.

The phase 1 computer simulation of the step response analysis consists of the error free analysis of both the linear and non-linear versions of all four reactor system cases. For each case, the magnitude of the step disturbance $A$ ranged up to $\pm 6^\circ$. For each amplitude of the step disturbance, the step response analysis was performed using 7, 10, 25, and 50 observations or measurements of the system response. Fourteen different values of $\Delta t$ were applied to each set of $N$ observations with the values of $\Delta t$ ranging in equal increments from 0.025 to 0.350 for Cases 1, 3, and 4, and from 0.0125 to 0.175 for Case 2. A set of typical results for the simulation of the step response of the linearized model is presented in Table II for the conditions given in the table. Results for the corresponding non-linear model are given in Table III.
The simulation of the step response analysis of the linear system with no measurement error provides an estimate of the best results which can be achieved with this method of transient response analysis. For Cases 1, 2, and 4 an upper limit on the value of $\Delta t$ was observed. Runs made with $\Delta t$ larger than the upper limit resulted in erroneous values for the imaginary part of the complex root, $b$, resulting in large values of the error criterion $S\psi$. It was further found that this maximum value of the time period between observations, $\Delta t_m$, is related to $b$ by:

$$\Delta t_m = \frac{\pi}{b}$$  \hspace{1cm} (70)

The observed values of $\Delta t_m$ and the values predicted by Equation (70) for Cases 1, 2, and 4 are shown in Table 4. Since the roots of the characteristic equation of the linear approximation of Case 3 are all real, no such limiting value of $\Delta t$ would be expected. This was found to be true since good results were obtained for Case 3 in the expanded range of values of $\Delta t$ from 0.075 to 0.450.

As long as the values of $\Delta t$ in Cases 1, 2, and 4 remain below the maximum value $\Delta t_m$, the values of the error criterion $S\psi$ were very near zero. Neither the number of observations $N$ nor the amplitude $A$ had any consistent effect on $S\psi$ in the analysis of the linear system. For very small values of the step amplitude $A$, $S\psi$ did increase somewhat. This effect is probably caused by round-off
error. For values of $\Delta t$ in the range from 0.0125 to 0.05, $\mathcal{S}_d$ appeared to be a function of the number of observations $N$. As $N$ increased, $\mathcal{S}_d$ decreased. It was concluded that only the first portion of the transient behavior was observed with these small values of $\Delta t$, and that observation of only this portion of the response was insufficient for determining the system parameters accurately. Within the limits of $\Delta t$ and $A$ prescribed above, however, the step response analysis of the linear system was essentially error free. This is indeed fortunate since the total value of $\mathcal{S}_d$ observed in phase 2, the step response analysis of the linear system with measurement error, can be attributed to the measurement error.

The upper limit $\Delta t_m$ observed in the simulation of the step response analysis of the linear system was also observed in the analysis of the non-linear system. This limit was approximately one time increment smaller than the maximum value for the linear system. Values of $\Delta t_m$ for the non-linear analysis are also tabulated in Table 4.

The non-linear effect should occur predominately as a function of the amplitude of the step disturbance. Generally, the larger the disturbance, the more non-linear the behavior of the system should become. The effect of the step amplitude on the non-linearity of the system can be studied independently from the method of analysis. Define $y_{NL_k}$, $k = 0, 1, ..., N-1$, as the set of discrete
observations of the response of the non-linear system to a step of amplitude \( A \). Also define \( y_{L_k} \), \( k = 0, 1, \ldots, N-1 \), as the set of discrete observations of the response of the linear system to a step of the same amplitude. If the \( N \) observations of the linear and non-linear responses are made with the same value of \( \Delta t \), the deviation of the system from linear behavior can then be described by the function:

\[
D = \frac{\left( \sum_{i=0}^{N-1} (y_{NL_i} - y_{L_i})^2 \right)^{\frac{1}{2}}}{\left( \sum_{i=0}^{N-1} (y_{NL_i})^2 \right)^{\frac{1}{2}}} \tag{71}
\]

Figure 1 is a plot of \( D \) versus amplitude \( A \) for Cases 1, 2, 3, and 4 with \( \Delta t \) constant for each case. From this plot, it is clear that Cases 1 and 2 do exhibit a high degree of non-linearity.

A measure of the non-linear effect of the amplitude \( A \) is also possible using the error criterion \(|S\Phi|\). A comparison of the two measures of the effect of step amplitude on the system non-linearity is possible if a plot of the absolute value \(|S\Phi|\) is made versus \( A \) over the same range of variables as the plot of \( D \) versus \( A \). Figure 2 is the plot of \(|S\Phi|\) versus \( A \) for Cases 1, 2, 3, and 4. No comparison of the magnitudes of \( D \) and \(|S\Phi|\) are possible, but
the fact that the plot of $\Psi$ agrees in form with the plot of $D$ adds weight to the validity of $\Psi$ as the criterion of error in this analysis. For positive values of the step of amplitude $A$, $\Psi$ for the non-linear system was positive, and for negative values of $A$, $\Psi$ was negative. The significance of this will be demonstrated later when the non-linear effects are combined with the measurement error effects.

The effect of the number of observations on $\Psi$ in the analysis of the non-linear system was not as pronounced or as consistent as the effect of the step amplitude $A$ or the value of $\Delta t$. Results for $N = 7$, the minimum number of observations were comparable to results for $N = 10, 25$, and $50$ for $\Delta t$ within the limits prescribed.

The second and third phases of this investigation are concerned with the effect of measurement error on the step response analysis of the linear and non-linear versions of the stirred tank reactor. The first group of runs made with measurement error followed the procedure of the runs made without measurement error. Thus the sequence of fourteen values of $\Delta t$ was applied to each set of $N$ observations.

From this group of runs it was found that measurement error reduced the upper limit of $\Delta t$ even more for both the linear and non-linear models. The ranges of allowable values of $\Delta t$ for Case 1, Case 2, and Case 4 respectively are $0.05-0.225$, $0.0375-0.1375$, and $0.025-0.175$. A value of
\( \Delta t \) was found from each of these sets of allowable values which gave consistently good results for \( N = 50 \) and for all amplitudes of the step \( A \) considered. This "optimal" value of \( \Delta t \) was found to be approximately 0.4 times the upper limit predicted by Equation (70). Values of \( \Delta t \) for Case 1, 2, and 3 are respectively 0.125, 0.075, and 0.1125.

No consistent behavior was observed in the simulation of the step response analysis of Case 3 with measurement error. The roots of the fitted model often included a complex pair whereas the roots of the linearized system for Case 3 were all real. It was felt that this problem was caused by limitations of the Prony method of analysis. It was thus concluded that this method is unsuitable for analysis of systems with all real roots in the presence of measurement error.

In the simulation of measurement error effects by superimposing random numbers on the calculated values of the system response, it is necessary to generate and apply as many of these numbers as possible so that the numbers can approach the properties of randomness assumed for them. Time and computer limitations make it impractical to generate and analyze systems in which over 200 observations of the system response are made. If \( \Delta t \) and \( N \) are held constant, it is convenient to calculate the response of the system to a step of amplitude \( A \), and then perform the step response analysis with this response subjected to a number of
independent sequences of random numbers. Thus further simulations of the step response analysis with measurement error were carried out with $\Delta t$ for each case set to the value given in a previous section and with $N$ equal to 50. The step response analysis was then simulated with the observations of the system response subjected to fourteen different sets of $N$ random numbers. Properties of the fourteen sequences of random numbers with $F = 0.0001$ are shown in Table 5. An average value $\overline{\mathcal{V}}$ was calculated from the fourteen resulting values of $\mathcal{V}$ and was used as a measure of the error effects on the step response analysis. Table 6 shows typical results for the simulation of the step response analysis of the linearized system with measurement error. Results from the corresponding non-linear system are given in Table 7.

The purpose of phase 2 of this investigation is to study the effects of measurement error alone on the step response analysis. It was discovered earlier that the step response analysis of the linear system, performed with certain restrictions on $\Delta t$, resulted in values of $\mathcal{V}$ that approached zero. The total value of $\overline{\mathcal{V}}_{\text{LE}}$ observed in the simulation of the step response analysis of the linear system should then be due only to measurement error superimposed on the response.

Since $N$ and $\Delta t$ are held constant in this series of runs, the measurement error is observed as a function of
the step amplitude \( A \). Figure 3 is a plot of \( \overline{\Psi}_{LE} \) versus 
\( A \) for Case 2 with measurement errors given by \( F \) in the range 
\(-0.0001 \leq 0 \leq 0.0001\). This behavior, in which \( \overline{\Psi}_{LE} \) is con-
sistently negative for both positive and negative step dis-
turbances, was observed for all cases when \( F/A \), the ratio 
of the measurement error to the step amplitude, was less 
than \( 10^{-3} \). This negative value observed for \( \overline{\Psi}_{LE} \) is verified 
by a relationship derived in Appendix A for estimating 
measurement error effects on the step response analysis of 
a linear system. The derivation is based on the step response 
analysis of a linear system when small random errors with a 
mean square value \( f_1^2 \) are superimposed on the observed values 
of the system step response. The derived expression is:

\[
\overline{\Psi}_{LE} = \frac{-f_1^2}{A^2} \cdot \frac{10^5}{2} \cdot T 
\]

(72)

where \( T \) is the period of observation:

\[
T = N \Delta t 
\]

(73)

Although Equation (72) shows that \( \overline{\Psi}_{LE} \) should be nega-
tive, values of \( \overline{\Psi}_{LE} \) calculated with the equation differ 
greatly from the observed values of \( \overline{\Psi}_{LE} \). This is shown 
in Figure 4 where observed and calculated values of \( \overline{\Psi}_{LE} \) 
are plotted versus the ratio \( f_1^2/A^2 \) for the linear system 
of Case 2.
In the derivation of Equation (72) for $\mathcal{S}\varphi_{LE}$, errors introduced in the method used to fit the observed data to the linear model were ignored. Appendix B shows that a large amplification of the measurement error can occur in one section of the Prony method. It further shows that this error amplification is greatest when the ratio $\frac{f_1^2}{A^2}$ is small, and that for the range of $\frac{f_1^2}{A^2}$ covered in Figure 4, the mean square observational error effect can grow sufficiently to give the differences between the observed and predicted values of $\mathcal{S}\varphi_{LE}$ seen.

Even though there is a large difference between the predicted value of $\mathcal{S}\varphi_{LE}$ and the observed value of $\mathcal{S}\varphi_{LE}$, $\mathcal{S}\varphi_{LE}$ should react to the variables $f_1^2$, $T$, and $A$ according to Equation (72). The following sections describe simulations of the step response which test this.

The effects of $T = N \Delta t$ on $\mathcal{S}\varphi_{LE}$ were investigated by performing the simulation of the step response analysis with $N = 100$ and $N = 200$ with constant $\Delta t$. Results from these runs along with results for $N = 50$ are shown in Table 8 for the conditions of Case 2 with measurement error given by $F = 0.0001$. In some cases $\mathcal{S}\varphi_{LE}$ is approximately proportional to $T$ as predicted by Equation (72). In all cases $\mathcal{S}\varphi_{LE}$ increases as $T$ increases.

To further investigate the effect of measurement error on the analysis of the linear system, simulations of the step response analysis were performed with the factor $F$ equal to
0.001, 0.01, 0.1 and 1.0 in addition to the runs made with F equal to 0.0001. Recall that the range of magnitudes of the measurement error is defined by \(-F \leq 0 \leq F\). These runs showed that the measurement error effect for a constant period of observation \(T\) was the same for any combination of \(F\) and \(A\) that resulted in a constant value of the ratio \(F/A\) or equivalently \(\frac{\bar{r}_1^2}{A^2}\). For the ratio \(F/A\) less than \(10^{-3}\), \(\bar{\Sigma}_0^{\perp}\) behaved according to Equation (72) in that it increased to large negative values as \(\frac{\bar{r}_1^2}{A^2}\) increased. This is shown in the plot in Figure 4 of \(\bar{\Sigma}_0^{\perp}\) versus \(\frac{\bar{r}_1^2}{A^2}\) for the conditions of Case 2 and in Table 9 which tabulates \(\bar{\Sigma}_0^{\perp}\) versus \(\frac{\bar{r}_1^2}{A^2}\) for Case 1.

For the ratio \(F/A\) greater than \(10^{-3}\), \(\bar{\Sigma}_0^{\perp}\) was no longer consistently negative and the measurement error effect could not be described in terms of \(\bar{\Sigma}_0^{\perp}\). The measurement error effect was then described by the mean square value of the error criterion, \(\bar{\Sigma}_0^{\perp}\). This representation of the measurement error effect was also found to remain constant for any combination of \(F\) and \(A\) that resulted in the same value of the ratio \(F/A\). The value \(\bar{\Sigma}_0^{\perp}\) was found to be approximately proportional to \((F/A)^2\). This is shown in Table 10 in which \(\bar{\Sigma}_0^{\perp}\) and \(\bar{\Sigma}_0^{\perp}/(F/A)^2\) are tabulated versus \(F/A\) for Case 2. The ratio \(\bar{\Sigma}_0^{\perp}/(F/A)^2\) for this case has a constant value of approximately \(3 \times 10^{-4}\).

Phase 3 of this investigation considers the combined effect of system non-linearity and measurement error on the
step response analysis of the stirred tank chemical reactor. This was done by simulating the step response analysis of the non-linear system with measurement errors superimposed on the response. It was found from these simulations that measurement error affects the step response analysis of the non-linear system in approximately the same manner it affects the analysis of the linear system.

In runs made with the ratio F/A less than $10^{-3}$, the combined effect of measurement error and system non-linearity is represented by $\Psi_{NLE}$. The value of $\Psi_{NLE}$ was found to approximately equal the sum of $\Psi_{NL}$, the effect of system non-linearity alone and $\Psi_{LE}$, the effect of measurement error alone. The effect of measurement error on the analysis of the non-linear system was thus approximately equal to $\Psi_{LE}$. This superposition property can be demonstrated by comparing the observed value of $\Psi_{NLE}$ with $\Psi_{NL+LE}$ obtained by adding $\Psi_{NL}$ and $\Psi_{LE}$. This is done in Tables 11, 12, and 13 for Cases 1, 2, and 4 respectively. Figure 5 is a plot of $\Psi_{NL}$, $\Psi_{LE}$, and $\Psi_{NLE}$ versus the step amplitude A. This plot also shows how the measurement error effects and non-linear effects combine for F/A less than $10^{-3}$.

Similar results were observed in runs made with F/A greater than $10^{-3}$. The effect of measurement error on the analysis of the non-linear system in this range of F/A is given by the mean square value of the difference between
\[ \Sigma \psi_{\text{NLE}} \] and \[ \Sigma \psi_{\text{NL}}. \] This quantity was observed to approximately equal the mean square value of \[ \Sigma \psi_{\text{LE}}. \] the effect of measurement error on the analysis of the linear system. The plot of \[ ( \Sigma \psi_{\text{NLE}} - \Sigma \psi_{\text{NL}})^2 \] and \[ \Sigma \psi_{\text{LE}}^2 \] versus \( (F/A)^2 \) for Case 2 in Figure 6 demonstrates this. Information concerning \[ \Sigma \psi_{\text{LE}}^2 \] for the linear system as a function of \( (F/A)^2 \) could therefore be used to predict measurement error effects on the analysis of the non-linear system.

For \( F/A \) less than \( 10^{-3} \), the minimum value of \[ \Sigma \psi_{\text{NLE}} \] occurs for the positive step disturbance for which the positive value of \[ \Sigma \psi_{\text{NL}} \] and the negative value of \[ \Sigma \psi_{\text{LE}} \] are of the same magnitude and cancel each other such that \[ \Sigma \psi_{\text{NLE}} \] approaches zero. This occurs in Figure 5 for Case 1 with \( F = 0.0001 \) at \( A = 0.2 \).

Measurement error and system non-linearity effects are minimized for \( F/A \) greater than \( 10^{-3} \) by the step amplitude \( A \) for which the sum of \[ \Sigma \psi_{\text{NL}}^2 \] and \[ \Sigma \psi_{\text{LE}}^2 \] is a minimum. The effect of system non-linearity on the step response analysis, \[ \Sigma \psi_{\text{NL}} \], is approximately proportional to the step amplitude \( A \). The measurement error effect, \[ \Sigma \psi_{\text{LE}}^2 \], is directly proportional to the ratio \( (F/A)^2 \). Further, since \[ \Sigma \psi_{\text{LE}} \] is the result of the cumulative effect of a large number of independent causes, the random measurement errors, the distribution of \[ \Sigma \psi_{\text{LE}} \] can be assumed normal. From this, the value of \[ \Sigma \psi_{\text{NLE}} \] can be predicted from \[ \Sigma \psi_{\text{NL}} \] as a function of \( A \) and from \[ \Sigma \psi_{\text{LE}} \] of a given probability as a function of \( (F/A)^2 \). With this
information the value of the step disturbance A can be found which results in the probable minimum value of $\frac{\sigma^2_{NLE}}{\text{range}}$ for the range of measurement errors given by $F$.

The purpose of this investigation was to study the effects of system non-linearity and measurement error on the transient response analysis of a chemical reactor system. It was also to determine whether some combination of the analysis parameters $\Delta t$, $A$, and $N$ minimizes the combined effect of system non-linearity and measurement error.

An absolute upper limit and an optimal range of values was found for $\Delta t$ as a function of the imaginary part of the complex roots of the characteristic equation of the linearized system. The effect of the number of observations $N$ on the step response analysis was observed to be insignificant compared to the effect of $\Delta t$ and $A$. In fact for the error free analysis, the only effect of increasing the number of samples from the minimum number of $N = 7$ to $N = 50$ was to increase the range of optimal $\Delta t$ to include smaller values of $\Delta t$.

The combination of $N = 50$ and $\Delta t = 0.125, 0.075, \text{and } 0.1125$ for Cases 1, 2, and 4 respectively was found to give consistently good results for the step response analysis conducted both with and without measurement error. For this reason, the studies of the effects of system non-linearity and measurement error on the step response analysis consist mostly of simulations with $\Delta t$ and $N$ at the above values. The results of these studies are summarized below.
1. The effect of system non-linearity on the step response analysis with no measurement error is represented by $\overline{\mathcal{L}} \varphi_{NL}$. The observed effects of system non-linearity are presented in the plot of the absolute value of $\overline{\mathcal{L}} \varphi_{NL}$ versus the step amplitude $A$ in Figure 2. The observed behavior is in accordance with the expected behavior since the non-linear effect becomes greater as the step amplitude increases. For the range of step amplitudes considered, the value of $\overline{\mathcal{L}} \varphi_{NL}$ is approximately proportional to the step amplitude and approaches zero for very small values of $A$. The effect of system non-linearity can then be represented by the slope of the plot of $\overline{\mathcal{L}} \varphi_{NL}$ versus the step amplitude $A$. Values of this proportionality constant for Cases 1, 2, and 4 are respectively 20.7, 0.85, and 0.125 for positive step disturbances.

2. The effect of measurement error alone was studied by simulating the step response analysis of the linear system with measurement error. A change in the mechanism of the error effect was observed over the range of measurement errors and step amplitudes considered. For small values of the ratio $F/A$ the measurement error effect $\overline{\mathcal{L}} \varphi_{LE}$ was consistently negative and could be represented by its mean value $\overline{\overline{\mathcal{L}} \varphi_{LE}}$ (Figure 3 and Table 6). The error criterion $\overline{\overline{\mathcal{L}} \varphi_{LE}}$ was found to be a non-linear function of $(F/A)^2$ rather than the linear function predicted by Appendix A and presented in Equation (72) (Figure 4 and Table 8). This
was caused by an amplification of the error effect that occurs in the Prony method which is also a function of \((F/A)^2\). This was shown in Appendix B.

The error effect for values of the ratio \(F/A\) greater than \(10^{-3}\) occurred in a more expected form. The error criterion \(\Sigma \Phi_{LE}\) was normally distributed about a zero mean with the mean square value \(\overline{\Sigma \Phi^2_{LE}}\) directly proportional to \((F/A)^2\) (Table 10).

3. The combined effect of measurement error and system non-linearity was studied by simulating the step response of the non-linear system with measurement error. Over the whole range of the ratio of \(F/A\) considered, it was found that the measurement error effect on the analysis of the non-linear system was approximately the same as the effect on the linear system. This is shown for values of \(F/A\) less than \(10^{-3}\) by the combination of \(\Sigma \Phi_{NL}\) with \(\Sigma \Phi_{LE}\) to give \(\overline{\Sigma \Phi_{NLE}}\) (Tables 11, 12 and 13 and Figure 5). For \(F/A\) greater than \(10^{-3}\) this is shown by the equality of \((\overline{\Sigma \Phi^2_{NLE}} - \Sigma \Phi^2_{NL})^2\) to \(\overline{\Sigma \Phi^2_{LE}}\) (Figure 6).

For \(F/A\) greater than \(10^{-3}\) the combined effect of system non-linearity and measurement error \(\overline{\Sigma \Phi^2_{NLE}}\) can be predicted from knowledge of \(\Sigma \Phi_{NL}\) as a function of \(A\) and from \(\overline{\Sigma \Phi^2_{LE}}\) as a function of \((F/A)^2\). The relationship between these is:

\[
\overline{\Sigma \Phi^2_{NLE}} = \Sigma \Phi^2_{NL} + \overline{\Sigma \Phi^2_{LE}}
\] (74)
For Case 2 the approximate relationship between $\bar{\delta \psi}_{NL}$ and A is given $\bar{\delta \psi}_{NL} = 0.85A$. The relationship between $\bar{\delta \psi}_{LE}^{2}$ and $(F/A)^2$ for the same case is $\bar{\delta \psi}_{LE}^{2} = 3(F/A)^2 \cdot 10^4$. Define $A_{opt}$ as the value of the step disturbance which results in the minimum value of $\bar{\delta \psi}_{NLE}^{2}$ for a given value of F. An expression for the value of $A_{opt}$ as a function of F can be obtained if it is assumed that Equation (74) and the relationships between $\bar{\delta \psi}_{NL}$ and A and between $\bar{\delta \psi}_{LE}^{2}$ and $(F/A)^2$ are valid in the neighborhood of $A_{opt}$. Substituting these expressions into Equation (74):

$$\bar{\delta \psi}_{NLE} = (0.85)^2 A^2 + 3(F/A)^2 \cdot 10^4. \quad (74a)$$

The minimum value of $\bar{\delta \psi}_{NLE}$ occurs for $\frac{\partial}{\partial A} (\bar{\delta \psi}_{NLE}) = 0$, for which:

$$A = A_{opt} = 14.3 \sqrt{F}. \quad (74b)$$

The value of $\bar{\delta \psi}_{NLE}$ at $A = A_{opt}$ is then:

$$\bar{\delta \psi}_{NLE} = 294.5F. \quad (74c)$$

The value of $A_{opt}$ for $F = 0.1$ is found from Equation (74b) to be 4.52 with the resulting minimum value of $\bar{\delta \psi}_{NLE} = 29.45$ given by Equation (74c). For $F = 1.0$, the minimum value of $\bar{\delta \psi}_{NLE}$ is 294.5 with $A_{opt} = 14.3$. 
IV. Summary

This investigation has examined a particular case of problems in systems analysis. The general purpose of this class of problems is to determine the dynamic properties of a process from observations of the behavior of the operating process or model of the process when disturbed by a test probe. The goal is to provide a description of the process dynamics which can be used to predict the response of the process to some driving function or disturbance.

The particular case treated in this investigation was the transient analysis of a non-linear process with observations of the process response to the test probe masked by measurement error. The effects of measurement error and system non-linearity on the description of the process dynamics obtained in the transient analysis of the "operating" system were studied. From this study it was intended that a basis for conducting a particular transient analysis would be found which could minimize the combined effects of measurement error and system non-linearity.

This study was conducted by digital computer simulation of the step response analysis of a stirred tank chemical reactor. "Observed" values of the response of the reactor were generated by numerical solution of the equations describing the system. Measurement errors in these observations were simulated by superimposing random numbers on the discrete values of the system response obtained from the numerical
solution. These observed values were fitted to the form of the step response of the reactor temperature given by a linearized description of the reactor system. The impulse response was then obtained from this. This description of the process dynamics can be used to predict the response of the reactor temperature to any disturbance or driving function in input temperature.

Since the impulse response of the linearized system was known, the fitted impulse response could be compared with it. The success of the transient analysis of the chemical reactor was measured by comparing the response of the reactor temperature predicted by the fitted impulse response with the response of the linearized system. The input temperature disturbance applied in this comparison was a random signal described by the spectral density function:

$$ \Phi_{ii}(s) = \frac{1}{(\alpha - s)(\alpha + s)} $$  \hspace{1cm} (75)

The mean square value of the reactor temperature resulting from this driving function is given by:

$$ \Phi = \frac{\overline{T^2}}{s} = \frac{1}{2\pi j} \int_{-j\infty}^{j\infty} G(s) \Phi_{ii}(s) G(-s) \, ds \quad (76) $$

where $G(s)$ is the linearized system transfer function which is the Laplace transform of the linearized system impulse response. A value of $\Phi$ was calculated for $G_1(s)$ the fitted transfer function and for $G(s)$ the linearized system.
transfer function. The error $S_Y$ was then the error in the mean square value of the temperature response predicted by the description of the system dynamics obtained from the transient analysis. A further test of the fit would be to compare the response predicted by the fitted system to the response of the actual non-linear system when both are driven by a random signal. The description of the random disturbance given by Equation (75) is not sufficient for calculating the response of the non-linear system, so only comparison of the response of the linear systems were made.

There were several reasons for choosing this method of comparing the response predicted by the fitted system to the response predicted by the linearized system. The response of a linear system to a random disturbance is conveniently described by one number, the mean square value of the response. The mean square value of the response of a linear system described by its transfer function, to a random signal described by its spectral density function, is easily calculated from tabulated solutions of the above integral. The random signal given by $\Phi_{11}(s)$ was chosen as a one parameter model of many random disturbances.

The purpose of this investigation was to study the effects of system non-linearity and measurement error on the step response analysis of the stirred tank chemical reactor. From this study it was intended that a basis for conducting the step response analysis would be found which could minimize the combined effects of measurement error
and system non-linearity. The results of this study will now be examined from the point of view of providing such a basis. This presentation assumes that the system to be analyzed is similar to the system treated in this investigation.

In performing the step response analysis of a system several conditions have to be chosen. These are $\Delta t$, the time spacing between observations of the system response; $N$, the total number of observations; and $A$, the amplitude of the step disturbance. A basis for conducting the step response analysis such that the effects of measurement error and system non-linearity are minimized consists of a basis for choosing these variables. Any basis for choosing these variables requires knowledge of the system dynamics, so that the approach to an optimal analysis of a system is an iterative or learning process. As knowledge of the system dynamics improves, the choice of these variables can more effectively minimize the effects of non-linearity and measurement error. The minimization of the effect of system non-linearity and measurement error was found to be predominantly a function of the step amplitude $A$. The choice of $\Delta t$ and $N$ was not as critical.

For the analysis of a system whose linearized description has a characteristic equation with roots occurring as a complex pair, a $\pm ib$, the choice of $\Delta t$ is related to $b$. In this investigation consistent results were obtained in
analyzing the non-linear system with measurement error with

\[ \Delta t = 0.4 \frac{\pi}{b} \]

No basis for choosing \( \Delta t \) was discovered for systems whose linearized system has a characteristic equation with all real roots.

A basis for the choice of the number of observations or equivalently the choice of the total period of observation was not investigated. In the early simulations it was found that for values of \( \Delta t \) chosen by the relationship above, \( N = 50 \) gave consistent results in the analysis of the non-linear system with measurement error. Since the effect of changing \( N \) from this value was found to be insignificant compared to the effect of the step amplitude \( A \), most of the simulations were run with \( N = 50 \).

The combined effects of system non-linearity and measurement error can be minimized by the choice of the step amplitude \( A \). As a basis for choosing this variable, both the error criterion due to measurement error alone and the error criterion due to system non-linearity alone must be known as a function of the step amplitude \( A \). Once this information is available the step amplitude \( A \) that minimizes the combined effects of non-linearity and measurement error can be easily calculated. The problem then is to obtain this information while performing the step response analysis of the non-linear system with measurement error.
In this investigation it was discovered that the error criterion due to system non-linearity above is approximately proportional to the step amplitude \( A \). In a range of measurement error magnitudes that is thought to be reasonable, it was found that the error criterion due to measurement error alone could be assumed to be normally distributed with a zero mean. The mean square value of this error criterion is inversely proportional to the square of the step amplitude for a constant range of measurement errors. It was also discovered that the measurement error effect on the step response analysis of the non-linear system was approximately the same as its effect on the analysis of the linear system. These observations provide a basis for obtaining the information necessary for choosing the step amplitude to minimize non-linear and measurement error effects on the step response analysis.

The system to be analyzed is assumed to behave in the manner described above. The mean value of the error criterion observed from repeated step response analysis of the non-linear system with measurement error with step \( A \) constant describes the effect of system non-linearity alone. The variance of the error criterion for a large number of analyses should describe the effect of measurement error alone. The proportionality constant relating the error criterion alone to the square of the step amplitude can then be obtained. The relationship for the error criterion due to non-linearity
alone as a function of the step amplitude is obtained by repeating this experiment at a different amplitude of the step disturbance. These two relationships can then be used to estimate the value of the step amplitude which will minimize the combined effect of system non-linearity and measurement error on the step response analysis. This approach is of course limited by the number of experiments necessary to remove bias from the average values calculated.
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<th>Case 3</th>
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<td>6.0</td>
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### Table 2

**Typical Results for the Step Response Analysis of a Linear System With No Measurement Error**

Case 2 \( A=1.0 \) \( N=50 \)

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Table 3

Typical Results for the Step Response Analysis
of a Non-linear System With No Measurement Error

Case 2    A=1.0    N=50.0

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<th>$\psi_n$</th>
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<td>0.01536</td>
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<td>301.03655</td>
<td>-1.03239</td>
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<td>0.00426</td>
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Table 4

Maximum Value of Time Spacing Between Observations

<table>
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<tr>
<th>Case</th>
<th>$b$</th>
<th>$\pi/b$</th>
<th>Linear System $\Delta t_m$</th>
<th>Non-linear System $\Delta t_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>i</td>
<td>10.285</td>
<td>0.30</td>
<td>0.300-.325</td>
<td>0.275-.325</td>
</tr>
<tr>
<td>2</td>
<td>17.166</td>
<td>0.18</td>
<td>0.175</td>
<td>0.1625-.175</td>
</tr>
<tr>
<td>4</td>
<td>10.878</td>
<td>0.29</td>
<td>0.25-.275</td>
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Table 5
Properties of Sequences of Random Numbers

\( N=50 \quad F=0.0001 \)

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<tr>
<th>Mean Value x 10^{-6}</th>
<th>Mean Square Value x 10^{-9}</th>
<th>Variance x 10^{-9}</th>
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</thead>
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<tr>
<td>-5.127</td>
<td>3.090</td>
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<td>-6.221</td>
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<tr>
<td>3.077</td>
<td>3.226</td>
<td>3.216</td>
</tr>
<tr>
<td>2.480</td>
<td>3.017</td>
<td>3.011</td>
</tr>
<tr>
<td>-6.781</td>
<td>3.905</td>
<td>3.859</td>
</tr>
<tr>
<td>4.281</td>
<td>3.187</td>
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<tr>
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<td>2.682</td>
<td>2.665</td>
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<tr>
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<td>3.128</td>
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<td>2.892</td>
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<td>12.193</td>
<td>3.344</td>
<td>3.196</td>
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</table>

Average: 0.354, 3.263, 3.301
### Table 6

Typical Results for the Step Response Analysis of a Linear System with Measurement Error

Case 2  \(A=1.0\)  \(N=50\)  \(F=0.0001\)

<table>
<thead>
<tr>
<th>(\Delta t)</th>
<th>(a)</th>
<th>(b)</th>
<th>(r_3)</th>
<th>(S\Psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0750</td>
<td>-12.06112</td>
<td>17.19131</td>
<td>-19.98707</td>
<td>-0.2200883</td>
</tr>
<tr>
<td>0.0750</td>
<td>-12.10237</td>
<td>17.23311</td>
<td>-29.82936</td>
<td>-0.2701205</td>
</tr>
<tr>
<td>0.0750</td>
<td>-12.06874</td>
<td>17.20840</td>
<td>-26.91722</td>
<td>-0.2521171</td>
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<tr>
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<td>-12.11186</td>
<td>17.21043</td>
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<td>-0.2689868</td>
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\(\bar{S}\Psi_{LE} = -0.2395243\)

<table>
<thead>
<tr>
<th>(\Delta t)</th>
<th>(c_0)</th>
<th>(c_1)</th>
<th>(c_2)</th>
<th>(c_3)</th>
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<tbody>
<tr>
<td>0.0750</td>
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<td>0.19809</td>
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### Table 7

Typical Results for the Step Response Analysis of a Non-linear System with Measurement Error

<table>
<thead>
<tr>
<th>Case 2</th>
<th>A=1.0</th>
<th>N=50</th>
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<td></td>
<td></td>
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<td>( b )</td>
<td>( r_3 )</td>
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\( \overline{\delta \Psi_{NLE}} = 0.6182942 \)

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<th>( c_1 )</th>
<th>( c_2 )</th>
<th>( c_3 )</th>
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</table>
Table 8

Effect of N on the Analysis of the Linear System with Measurement Error for Case 2

\( F=0.0001, \ \Delta t=0.075 \)

<table>
<thead>
<tr>
<th>A</th>
<th>( \bar{Y}_{LE} ) for N=50</th>
<th>( \bar{Y}_{LE} ) for N=100</th>
<th>( \bar{Y}_{LE} ) for N=200</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.2391</td>
<td>-0.3214</td>
<td>-</td>
</tr>
<tr>
<td>0.2</td>
<td>-0.2080</td>
<td>-</td>
<td>-0.3460</td>
</tr>
<tr>
<td>1.0</td>
<td>-0.2395</td>
<td>-0.3548</td>
<td>-</td>
</tr>
<tr>
<td>2.0</td>
<td>-0.1910</td>
<td>-0.3372</td>
<td>-0.4094</td>
</tr>
<tr>
<td>4.0</td>
<td>-0.0774</td>
<td>-0.1915</td>
<td>-0.3203</td>
</tr>
<tr>
<td>10.0</td>
<td>-0.0132</td>
<td>-0.0380</td>
<td>-0.0881</td>
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</tbody>
</table>
Table 9

Error Criterion $\overline{\frac{\bar{\psi}_{\text{LE}}}{f_1^2/A^2}}$ as a Function of the Ratio $\frac{f_1^2}{A^2}$ for Case 1

N=50, $\Delta t=0.125$

<table>
<thead>
<tr>
<th>$\frac{f_1^2}{A^2}$</th>
<th>$\overline{\frac{\bar{\psi}_{\text{LE}}}{f_1^2/A^2}}$</th>
<th>$\overline{\frac{\bar{\psi}_{\text{LE}}}{f_1^2/A^2}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2.512 \times 10^{-11}$</td>
<td>-0.0204</td>
<td>-8.109 $\times 10^{8}$</td>
</tr>
<tr>
<td>$7.987 \times 10^{-11}$</td>
<td>-0.0553</td>
<td>-6.924 $\times 10^{8}$</td>
</tr>
<tr>
<td>$1.689 \times 10^{-10}$</td>
<td>-0.1096</td>
<td>-6.489 $\times 10^{8}$</td>
</tr>
<tr>
<td>$5.685 \times 10^{-10}$</td>
<td>-0.3485</td>
<td>-6.130 $\times 10^{9}$</td>
</tr>
<tr>
<td>$2.556 \times 10^{-9}$</td>
<td>-1.4387</td>
<td>-5.629 $\times 10^{8}$</td>
</tr>
<tr>
<td>$8.113 \times 10^{-9}$</td>
<td>-3.4497</td>
<td>-4.252 $\times 10^{8}$</td>
</tr>
<tr>
<td>$1.718 \times 10^{-8}$</td>
<td>-4.7844</td>
<td>-2.785 $\times 10^{8}$</td>
</tr>
<tr>
<td>$5.685 \times 10^{-8}$</td>
<td>-5.2802</td>
<td>-0.929 $\times 10^{8}$</td>
</tr>
<tr>
<td>$2.512 \times 10^{-7}$</td>
<td>-5.1840</td>
<td>-2.064 $\times 10^{7}$</td>
</tr>
<tr>
<td>$8.113 \times 10^{-7}$</td>
<td>-4.5059</td>
<td>-5.554 $\times 10^{6}$</td>
</tr>
<tr>
<td>$1.689 \times 10^{-6}$</td>
<td>-4.3908</td>
<td>-8.357 $\times 10^{5}$</td>
</tr>
<tr>
<td>$5.685 \times 10^{-6}$</td>
<td>-4.7509</td>
<td>-2.451 $\times 10^{5}$</td>
</tr>
<tr>
<td>$2.512 \times 10^{-5}$</td>
<td>-6.1578</td>
<td>-1.028 $\times 10^{5}$</td>
</tr>
<tr>
<td>$8.113 \times 10^{-5}$</td>
<td>-8.3414</td>
<td>-6.256 $\times 10^{4}$</td>
</tr>
<tr>
<td>$1.689 \times 10^{-4}$</td>
<td>-10.5662</td>
<td>-1.617 $\times 10^{4}$</td>
</tr>
</tbody>
</table>

(1) According to Equation (72) the value of this ratio should be $-3.125 \times 10^{5}$ for N=50, $\Delta t=0.125$. 
Table 10

ERROR CRITERION $\bar{\psi}_{LE}^2$ AS A FUNCTION OF THE RATIO $(F/A)^2$ FOR CASE 2

$N = 50 \quad \Delta t = .075$

<table>
<thead>
<tr>
<th>F/A</th>
<th>$\bar{\psi}_{LE}^2$</th>
<th>$\bar{\psi}_{LE}^2/(F/A)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0200</td>
<td>12.819</td>
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<tr>
<td>0.0250</td>
<td>19.443</td>
<td>$3.111 \times 10^4$</td>
</tr>
<tr>
<td>0.0333</td>
<td>33.077</td>
<td>$2.978 \times 10^4$</td>
</tr>
<tr>
<td>0.0500</td>
<td>76.129</td>
<td>$3.045 \times 10^4$</td>
</tr>
<tr>
<td>0.200</td>
<td>1336.8</td>
<td>$3.342 \times 10^4$</td>
</tr>
<tr>
<td>0.250</td>
<td>2114.6</td>
<td>$3.382 \times 10^4$</td>
</tr>
<tr>
<td>0.333</td>
<td>3853.8</td>
<td>$3.469 \times 10^4$</td>
</tr>
<tr>
<td>0.500</td>
<td>9349.9</td>
<td>$3.740 \times 10^4$</td>
</tr>
</tbody>
</table>
Table 11

<table>
<thead>
<tr>
<th>A</th>
<th>( S^\psi_{NL} )</th>
<th>( S^\psi_{LE} )</th>
<th>( S^\psi_{NLE} )</th>
<th>( S^\psi_{NL+LE} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0557</td>
<td>+0.904</td>
<td>-4.431</td>
<td>-3.679</td>
<td>-3.527</td>
</tr>
<tr>
<td>0.2957</td>
<td>+6.198</td>
<td>-4.980</td>
<td>+1.005</td>
<td>+1.218</td>
</tr>
<tr>
<td>0.5957</td>
<td>+12.346</td>
<td>-3.732</td>
<td>+8.217</td>
<td>+8.614</td>
</tr>
<tr>
<td>2.3957</td>
<td>+43.619</td>
<td>-0.348</td>
<td>+43.575</td>
<td>+43.271</td>
</tr>
<tr>
<td>4.3957</td>
<td>-78.869</td>
<td>-0.110</td>
<td>+78.849</td>
<td>+78.759</td>
</tr>
<tr>
<td>6.3957</td>
<td>+111.764</td>
<td>-0.055</td>
<td>+111.731</td>
<td>+111.709</td>
</tr>
</tbody>
</table>

Table 12

<table>
<thead>
<tr>
<th>A</th>
<th>( S^\psi_{NL} )</th>
<th>( S^\psi_{LE} )</th>
<th>( S^\psi_{NLE} )</th>
<th>( S^\psi_{NL+LE} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.020</td>
<td>-0.239</td>
<td>-0.274</td>
<td>-0.259</td>
</tr>
<tr>
<td>0.4</td>
<td>+0.122</td>
<td>-0.247</td>
<td>+0.026</td>
<td>-0.125</td>
</tr>
<tr>
<td>1.0</td>
<td>+0.616</td>
<td>-0.240</td>
<td>+0.618</td>
<td>+0.376</td>
</tr>
<tr>
<td>1.4</td>
<td>+1.000</td>
<td>-0.233</td>
<td>+1.001</td>
<td>+0.767</td>
</tr>
<tr>
<td>2.0</td>
<td>+1.570</td>
<td>-0.191</td>
<td>+1.568</td>
<td>+1.379</td>
</tr>
<tr>
<td>3.0</td>
<td>+2.485</td>
<td>-0.121</td>
<td>+2.484</td>
<td>+2.364</td>
</tr>
<tr>
<td>4.0</td>
<td>+3.354</td>
<td>-0.077</td>
<td>+3.354</td>
<td>+3.277</td>
</tr>
<tr>
<td>5.0</td>
<td>+4.182</td>
<td>-0.052</td>
<td>+4.181</td>
<td>+4.130</td>
</tr>
</tbody>
</table>
Table 13

$\xi_{NL}$, $\xi_{LE}$, $\xi_{NLE}$, and $\xi_{NL+LE}$ for Case 4

$F = 0.0001$, $\Delta t = 0.1125$, $N = 50$

<table>
<thead>
<tr>
<th>A</th>
<th>$\xi_{NL}$</th>
<th>$\xi_{LE}$</th>
<th>$\xi_{NLE}$</th>
<th>$\xi_{NL+LE}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.048</td>
<td>-0.401</td>
<td>-0.457</td>
<td>-0.449</td>
</tr>
<tr>
<td>0.4</td>
<td>-0.005</td>
<td>-0.105</td>
<td>-0.112</td>
<td>-0.110</td>
</tr>
<tr>
<td>1.0</td>
<td>+0.081</td>
<td>-0.110</td>
<td>-0.034</td>
<td>-0.029</td>
</tr>
<tr>
<td>1.4</td>
<td>+0.138</td>
<td>-0.101</td>
<td>+0.033</td>
<td>+0.037</td>
</tr>
<tr>
<td>2.0</td>
<td>+0.222</td>
<td>-0.062</td>
<td>+0.159</td>
<td>+0.159</td>
</tr>
<tr>
<td>3.0</td>
<td>+0.357</td>
<td>-0.064</td>
<td>+0.296</td>
<td>+0.294</td>
</tr>
<tr>
<td>4.0</td>
<td>+0.493</td>
<td>-0.049</td>
<td>+0.445</td>
<td>+0.443</td>
</tr>
<tr>
<td>5.0</td>
<td>+0.622</td>
<td>-0.036</td>
<td>+0.589</td>
<td>+0.585</td>
</tr>
</tbody>
</table>
Fig. 1 System deviation from linear behavior vs step amplitude
Fig. 2 Absolute value of error criterion for analysis of non-linear system vs step amplitude
Fig. 3  Error criterion for analysis of linear system with measurement error vs step amplitude for case 2
\[ \Delta t = 0.075 \quad \delta = 0.0001 \quad N = 50 \]
Fig. 4  Observed and predicted linear system measurement error effects vs. ratio \( \frac{f_i^2}{A^2} \) for case 2
Fig. 5  Error criteria $\delta \varphi_{NL}, \bar{\delta \varphi}_{LE}, \bar{\delta \varphi}_{NLE}$ vs. step amplitude for case 1
$\Delta t = 0.125$  $F = 0.0001$  $N = 50$
$A_0 = \frac{8e_0^2}{\Delta}$

$\Delta = (8\Phi_{NLE} - 8\Phi_{NL})^2$

$10^{-2}$

$10^{-3}$

$10^{-1}$

$10^2$

$10^3$

$10^4$

Fig. 6: Observed linear $\beta$, non-linear system measurement error effect vs. $(F/A)^2$ for case 2
Appendix A

An Estimate of the Effect of Measurement Error on the Step Response Analysis of a Linear System

Consider the general fourth order linear system:

\[ \frac{dx}{dt} = Bx + Ez. \tag{A.1} \]

The transient response of the system to a step disturbance in \( z \) is given by the numerical approximation:

\[ \frac{x^{n+1} - x^n}{\Delta t} = \frac{E(x^{n+1} + x^n)}{2} + Ez \tag{A.2} \]

\[ (I - \frac{\Delta t}{2} B)x^{n+1} = (I + \frac{\Delta t}{2} B)x^n + tEz \tag{A.3} \]

Let \( C = (I - \frac{\Delta t}{2} B)^{-1} (I + \frac{\Delta t}{2} B), \tag{A.4} \)

\[ D = (I - \frac{\Delta t}{2} B)^{-1} \Delta tE, \tag{A.5} \]

so that

\[ x^{n+1} = Cx^n + Dz. \tag{A.6} \]

Measure time from the application of the step and assume that the state variables \( (x_1, x_2, x_3, x_4) \) have been defined such that \( x = x^0 = 0 \) at \( t = 0 \). Then, for \( n > 0 \)

\[ x^n = \sum_{k=1}^{n} C^{n-k} Dz \tag{A.7} \]
A simple relationship exists between the step response $x$ and the system unit impulse response $g$. Thus, if the disturbance is restricted to a step of amplitude $A$ in any one element of the vector $z$, the unit impulse response $g$ is:

$$ g = \frac{1}{A} \frac{dx}{dt}, \quad (A.8) $$

or

$$ g^n = \frac{1}{A} \frac{x^{n+1} - x^{n-1}}{2 \Delta t}, \quad (A.9) $$

$$ g^n = \frac{1}{A} \left[ \frac{Dz}{\Delta t} \right]^{n-1} \quad (A.10) $$

Suppose that each observation of the step response vector $x$ includes a vector of random measurement errors $f$ superimposed on it. Designating the observed values of the response vector by $x^{n'}$, the true values by $x^n$, and the errors by $f^n$ yields:

$$ x^{n'} = x^n + f^n. \quad (A.11) $$

The impulse response $g^{n'}$ found from the step response with measurement error is then:

$$ g^{n'} = \frac{1}{A} \frac{x^{n+1} + f^{n+1} - x^{n-1} - f^{n-1}}{2 \Delta t}, \quad (A.12) $$

$$ g^{n'} = g^n + \frac{f^{n+1} - f^{n-1}}{2 \Delta t} \cdot (A.13) $$

An error criterion $\mathcal{S}\Phi$ was defined as:

$$ \mathcal{S}\Phi = (\Phi - \Phi_1) 10^5, \quad (A.14) $$
\[ \Phi_1 = \frac{1}{2\pi j} \int_{-\infty}^{\infty} G_1(s) \overline{\Phi}_{ii}(s) G_1(-s) \, ds, \]  
\[ \Phi = \frac{1}{2\pi j} \int_{-\infty}^{\infty} G(s) \overline{\Phi}_{ii}(s) G(-s) \, ds. \]  

(A.15)  

(A.16)

The transfer function of the linear system is \( G(s) \), and the transfer function of the system obtained from the step response analysis with measurement error is \( G_1(s) \). The driving function \( \overline{\Phi}_{ii}(s) \) is given by:

\[ \overline{\Phi}_{ii}(s) = \frac{-1}{s^2 - \lambda^2}. \]  

(A.17)

An equivalent time domain expression for the mean square value of the response \( \Phi \) is given by:

\[ \Phi = \int_0^\infty g(\tau) d\tau \int_0^\infty g(\sigma) d\sigma \phi_{ii}(\tau - \sigma) \]  

(A.18)

where \( \phi_{ii}(\tau - \sigma) \) is the autocorrelation function corresponding to \( \overline{\Phi}_{ii}(s) \):

\[ \phi_{ii}(\tau) = \frac{e^{-\lambda|\tau|}}{2\lambda} \]  

(A.19)

It is desirable to derive an expression for \( \Phi \) with the impulse response of the linear system approximated by \( g^n \) and the impulse response of the fitted system approximated by \( g'^n \). It is convenient to derive this expression in terms of \( g^n_1 \) since the procedure is identical for \( g^n_1, g^n_2, g^n_3, \) and \( g^n_4 \).

Define \( \tau = k \Delta t \),

(A.20)
\[ \sigma = n \Delta t \] \hspace{1cm} (A.21)

and the mean square value of the system response to \( \phi_{i1}(\tau) \) becomes:

\[ \varphi_1 = \lim_{N \to \infty} \frac{1}{2\alpha} \sum_{k=1}^{N} g_{i1}^k \Delta t \sum_{n=1}^{N} g_{i1}^n \Delta t e^{-\alpha|k-n|\Delta t} \] \hspace{1cm} (A.22)

For the linear system obtained from the step response analysis with measurement error:

\[ \varphi_{1,1} = \lim_{N \to \infty} \frac{1}{2\alpha} \sum_{k=1}^{N} g_{i1}^{k'} \Delta t \sum_{n=1}^{N} g_{i1}^{n'} \Delta t e^{-\alpha|k-n|\Delta t} \] \hspace{1cm} (A.23)

Expanding:

\[ \varphi_{1,1} = \lim_{N \to \infty} \frac{1}{2\alpha} \left\{ \sum_{k=1}^{N} g_{i1}^k \Delta t \sum_{n=1}^{N} g_{i1}^n \Delta t e^{-\alpha|k-n|\Delta t} \right\} \]

\[ + 2 \sum_{k=1}^{N} g_{i1}^k \Delta t \sum_{n=1}^{N} \frac{r_{i1}^{n+1} - r_{i1}^{n-1} e^{-\alpha|k-n|\Delta t}}{2A} \]

\[ + \frac{1}{4A^2} \left[ \sum_{k=1}^{N} r_{i1}^{k+1} \sum_{n=1}^{N} r_{i1}^{n+1} e^{-\alpha|k-n|\Delta t} \right. \]

\[ - 2 \sum_{k=1}^{N} r_{i1}^{k-1} \sum_{n=1}^{N} r_{i1}^{n+1} e^{-\alpha|k-n|\Delta t} \]

\[ + \sum_{k=1}^{N} r_{i1}^{k-1} \sum_{n=1}^{N} r_{i1}^{n-1} e^{-\alpha|k-n|\Delta t} \} \] \hspace{1cm} (A.24)
Expanding the term
\[ \sum_{k=1}^{N} f_{k+1}^{k+1} \sum_{n=1}^{N} f_{n+1}^{n+1} e^{-\alpha |k-n|} \Delta t \]
and collecting factors of like powers of the exponential gives:
\[ \sum_{k=1}^{N} f_{k+1}^{k+1} \sum_{n=1}^{N} f_{n+1}^{n+1} e^{-\alpha |k-n|} \Delta t = \sum_{q=1}^{N} f_{1}^{q+1} f_{1}^{q+1} \]
\[ + 2 \sum_{p=1}^{N-1} e^{-\alpha |p|} \Delta t \sum_{q=1}^{N-p} f_{1}^{q+1} f_{1}^{q+1+p}. \quad (A.25) \]

Similarly,
\[ \sum_{k=1}^{N} f_{1}^{k-1} \sum_{n=1}^{N} f_{1}^{n-1} e^{-\alpha |k-n|} \Delta t = \sum_{q=1}^{N} f_{1}^{q-1} f_{1}^{q-1} \]
\[ + 2 \sum_{p=1}^{N-1} e^{-\alpha |p|} \Delta t \sum_{q=1}^{N-p} f_{1}^{q-1} f_{1}^{q-1+p}. \quad (A.26) \]

And,
\[ \sum_{k=1}^{N} f_{1}^{k-1} \sum_{n=1}^{N} f_{1}^{n+1} e^{-\alpha |k-n|} \Delta t = \sum_{q=1}^{N-1} f_{1}^{q+1} f_{1}^{q} e^{-\alpha \Delta t} \]
\[ + \sum_{p=0}^{N-1} e^{-\alpha |p|} \Delta t \sum_{q=1}^{N-p} f_{1}^{q-1} f_{1}^{q+1+p} + \sum_{q=1}^{N-2} f_{1}^{q+1} f_{1}^{q+1} e^{-2\alpha \Delta t} \]
(cont.)
\[ + \sum_{p=3}^{N-1} e^{-\alpha \Delta t} \sum_{q=1}^{N-p} f_{i}^{q+1} f_{i}^{q-1+p}. \quad (A.27) \]

Now,
\[ \lim_{N \to \infty} \sum_{k=1}^{N} \frac{f_{k+u} f_{k+m}}{N} = 0, \quad u \neq m, \quad (A.28) \]
\[ = f_{i}^{m}, \quad u = m. \quad (A.29) \]

Then,
\[ \lim_{N \to \infty} \sum_{q=1}^{N} f_{i}^{q+1} f_{i}^{q+1} = N f_{i}^{2}, \quad (A.30) \]
\[ \lim_{N \to \infty} \sum_{q=1}^{N} f_{i}^{q-1} f_{i}^{q-1} = N f_{i}^{2}, \quad (A.31) \]

and
\[ \lim_{N \to \infty} \sum_{q=1}^{N-2} f_{i}^{q+1} f_{i}^{q+1} e^{-2\alpha \Delta t} = N f_{i}^{2} e^{-2\alpha \Delta t}. \quad (A.32) \]

Consider the remaining terms in (A.25), (A.26), and (A.27) which are of the form:
\[ \sum_{p=1}^{N-l} e^{-\alpha \Delta t} \sum_{q=1}^{N-p} f_{i}^{q+v} f_{i}^{q+w+p}, \quad q + v \neq q + w + p. \quad (A.33) \]

For \( p = u, \ u \ll N \) the limit can be written:
\[ \lim_{N \to \infty} N e^{-\alpha \Delta t} \sum_{q=1}^{N} f_{i}^{q+v} f_{i}^{q+w+u} = 0 \quad (A.34) \]
because of (A.28). Furthermore, for \( p = u, u \rightarrow N, N \rightarrow \infty \):
\[
e^{-\alpha |u| \Delta t} \rightarrow 0
\]  \hspace{1cm} (A.35)

and the terms are bounded. Thus as \( N \rightarrow \infty \) these terms become negligible compared to:
\[
\frac{\overline{N} f_i}{4 \alpha A^2} (1 - e^{-2\alpha \Delta t})
\]  \hspace{1cm} (A.36)

The term:
\[
\sum_{k=1}^{N} g_1^k \Delta t \sum_{n=1}^{N} \frac{f_i^{n+1} - f_i^{n-1}}{2A} e^{-\alpha |k-n| \Delta t}
\]  \hspace{1cm} (A.37)

is also negligible compared to (A.36) as \( N \rightarrow \infty \) since:
\[
g_1^k \rightarrow 0, \quad k \rightarrow N, \quad N \rightarrow \infty
\]  \hspace{1cm} (A.38)

and the terms \( f_i^{n+1} - f_i^{n-1} \) and \( e^{-\alpha |k-n| \Delta t} \) are bounded.

The error criterion as \( N \rightarrow \infty \) is then:
\[
\frac{S \varphi_i}{N \rightarrow \infty} = \frac{-\overline{N} f_i}{4 \alpha A^2} (1 - e^{-2\alpha \Delta t}) 10^5
\]  \hspace{1cm} (A.39)

As \( \Delta t \rightarrow C \) this becomes:
\[
\frac{S \varphi_i}{N \rightarrow \infty} = \frac{-\overline{N} f_i}{4 \alpha A^2} (2\alpha \Delta t) 10^5 = \frac{-f_i}{A^2} \frac{10^5}{2} T, \quad (A.40)
\]

where \( T = N \Delta t \) is the sampling period.
Appendix B

Error Analysis of Prony Method

The purpose of this section is to show how errors in observing the system step response can grow in fitting the observed data to the linear model using the Prony method. The error growth that occurs at each step of the Prony method will be examined.

The following is a typical example of the disagreement between observed and predicted values of the error criterion $S\Psi$. In the simulation of the step response analysis of the linear version of Case 2 with measurement error, the observed value of the error criterion with $A = 2.0$, $\Delta t = .075$, $N = 50$, and $F = 0.0001$ was $S\Psi_{LE} = -0.1910$. For these conditions $f_1 = 3.264 \times 10^{-9}$, and using the equation derived in Appendix A:

$$S\Psi = \frac{-f_1^2}{A^2} \frac{10^5}{2} T$$  \hspace{1cm} (B.1)

the value of $S\Psi$ is estimated to be $S\Psi = -0.1530 \times 10^3$. The observed value of $S\Psi$ is approximately $10^3$ times the predicted value. Another way to consider this error growth is to calculate the "effective" mean square error (which will be designated by $n_1^2$) necessary to cause the predicted value of the error criterion to be $S\Psi = -0.1910$. This was found to be $n_1^2 = 4.0187 \times 10^{-6}$ which is approximately $10^3$. 
times the actual mean square error \( \overline{e_i^2} \). It will be shown that this error amplification occurs in one step of the method used to fit the observed data to the linear model.

To simplify following the error effect through the Prony fit, the effect of a single error \( \varepsilon \) in observing the \( i \)th element of the step response will be considered. The \( i \)th element of the step response is given by:

\[
y_i' = y_i + \varepsilon \quad \text{(B.2)}
\]

where \( y_i' \) is the observed value, \( y_i \) is the true value, and \( \varepsilon \) is the error.

The first step in fitting the observed data to the linear model:

\[
y(t) = c_0 + \sum_{j=1}^{3} c_j e^{a_j t} \quad \text{(B.3)}
\]

consists of solving the following set of \( N-4 \) equations for \( \alpha_1, \alpha_2, \) and \( \alpha_3 \):

\[
\sum_{k=1}^{3} \alpha_k \Delta y_{j-k} = \Delta y_j \quad j = 3, 4, ..., N-2 \quad \text{(B.4)}
\]

with \( \Delta y_j = y_{j+1} - y_j \).

Because of the error \( \varepsilon \) in observing the \( i \)th element of the step response:

\[
\Delta y_i' = y_{i+1} - y_i - \varepsilon = \Delta y_i - \varepsilon \quad \text{(B.6)}
\]

\[
\Delta y_{i-1}' = y_i + \varepsilon - y_{i-1} = \Delta y_{i-1} + \varepsilon \quad \text{(B.7)}
\]
Equation (B.4) with the single measurement error $\varepsilon$ occurring in the observation of the $ith$ value of the step response becomes:

\[
\begin{bmatrix}
\Delta y_2 & \Delta y_1 & \Delta y_0 \\
\Delta y_3 & \Delta y_2 & \Delta y_1 \\
\vdots & \vdots & \vdots \\
\Delta y_{i-2} & \Delta y_{i-3} & \Delta y_{i-4} \\
\Delta y_{i-1} + \varepsilon & \Delta y_{i-2} & \Delta y_{i-3} \\
\Delta y_{i-1} & \Delta y_{i-1} + \varepsilon & \Delta y_{i-2} \\
\Delta y_{i+1} & \Delta y_{i-1} - \varepsilon & \Delta y_{i+1} + \varepsilon \\
\vdots & \vdots & \vdots \\
\Delta y_{N-3} & \Delta y_{N-4} & \Delta y_{N-5}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 + \varepsilon \\
\alpha_2 + \varepsilon \\
\alpha_3 + \varepsilon \\
\vdots \\
\Delta y_{i-1} + \varepsilon \\
\Delta y_{i-1} \\
\Delta y_{i+1} \\
\Delta y_{i+2} \\
\Delta y_{i+3} \\
\vdots \\
\Delta y_{N-2}
\end{bmatrix}
= 
\begin{bmatrix}
\Delta y_3 \\
\Delta y_4 \\
\vdots \\
\Delta y_{i-1} + \varepsilon \\
\Delta y_{i-1} \\
\Delta y_{i+1} \\
\Delta y_{i+2} \\
\Delta y_{i+3} \\
\vdots \\
\Delta y_{N-2}
\end{bmatrix}
\]  

(B.8)

where $\varepsilon \alpha_k$ is the error in the calculated value of $\alpha_k$ resulting from the measurement error.

The normalized set of equations in the least squares solution of Equation (B.4) is:

\[
\sum_{k=1}^{3} \alpha_k \sum_{j=3}^{N-2} \Delta y_{j-k} \Delta y_{j-r} = \sum_{j=3}^{N-2} \Delta y_{j} \Delta y_{j-r}, \ r=1,2,3,
\]  

(B.9)
or
\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3
\end{bmatrix}
= 
\begin{bmatrix}
q_1 \\
q_2 \\
q_3
\end{bmatrix}
\] (B.10)

For this case it was found that first order terms in \( \varepsilon \) are small compared to the second order terms. Then Equation (B.10) with measurement error becomes:
\[
\begin{bmatrix}
a_{11} + 2 \varepsilon & a_{12} - \varepsilon & a_{13} \\
a_{21} & a_{22} + 2 \varepsilon & a_{23} - \varepsilon \\
a_{31} & a_{32} & a_{33} + 2 \varepsilon
\end{bmatrix}
\begin{bmatrix}
\alpha_1 + \delta \alpha_1 \\
\alpha_2 + \delta \alpha_2 \\
\alpha_3 + \delta \alpha_3
\end{bmatrix}
= 
\begin{bmatrix}
q_1 - \varepsilon \\
q_2 \\
q_3
\end{bmatrix}
\] (B.11)

It was also found for this case that products of the type \( \varepsilon^2 \delta \alpha_k \) are negligible. Substracting (B.10) from (B.11) gives:
\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix}
\begin{bmatrix}
\delta \alpha_1 \\
\delta \alpha_2 \\
\delta \alpha_3
\end{bmatrix}
= 
\begin{bmatrix}
\varepsilon^2 (\alpha_2 - 2 \alpha_1 - 1) \\
\varepsilon^2 (\alpha_1 - 2 \alpha_2 + \alpha_3) \\
\varepsilon^2 (\alpha_2 - 2 \alpha_3)
\end{bmatrix}
\] (B.12)

The values of \( a_{rk} \) and \( \alpha_k \) are known so that Equation (B.12) can be solved for \( \delta \alpha_1 \), \( \delta \alpha_2 \), and \( \delta \alpha_3 \) in terms of the single measurement error:
\[
\delta \alpha_1 = -2.381 \varepsilon^2 \times 10^6,
\delta \alpha_2 = 5.303 \varepsilon^2 \times 10^5,
\delta \alpha_3 = -3.828 \varepsilon^2 \times 10^5.
\] (B.13)
The error amplification that takes place here is caused by the small value of the determinant of the matrix of coefficients in Equation (B.12). This determinant has the value of $D_1 = 7.3 \times 10^{-7}$.

For the case that is being examined $A = 2.0$, $\overline{f_1^2}/A^2 = 3.264 \times 10^{-9}$ so that $\overline{f_1^2}/A^2 = 8.16 \times 10^{-10}$. As the value of the ratio $\overline{f_1^2}/A^2$ increases from this, the value of the determinant $D_1$ increases. This causes the error growth to decrease as $\overline{f_1^2}/A^2$ increases. The behavior of the determinant $D_1$ as a function of $\overline{f_1^2}/A^2$ is seen in the following tabulation of observed values of $\overline{f_1^2}/A^2$ and $D_1$.

<table>
<thead>
<tr>
<th>$\overline{f_1^2}/A^2$</th>
<th>$D_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7.3 x $10^{-7}$</td>
</tr>
<tr>
<td>$8.16 \times 10^{-10}$</td>
<td>9.4 x $10^{-7}$</td>
</tr>
<tr>
<td>$8.16 \times 10^{-8}$</td>
<td>1.57 x $10^{-5}$</td>
</tr>
<tr>
<td>$8.16 \times 10^{-6}$</td>
<td>1.46 x $10^{-3}$</td>
</tr>
<tr>
<td>$8.16 \times 10^{-4}$</td>
<td>.4087</td>
</tr>
</tbody>
</table>

Note that the value of $D_1$ for $\overline{f_1^2}/A^2 = 8.16 \times 10^{-10}$ has not changed greatly from the value of the error free determinant. For $\overline{f_1^2}/A^2$ greater than $8.16 \times 10^{-10}$, the increase in $D_1$ is approximately proportional to the increase in $\overline{f_1^2}/A^2$. This increase in the value of the determinant for $\overline{f_1^2}/A^2 > 8.16 \times 10^{-10}$ is caused by error effects which were ignored in the development of Equation (B.12). No simple relationship could be derived to predict the effects of these terms. Further evidence of the decrease in the error growth with an increase in $\overline{f_1^2}/A^2$ will be presented later in this section.
The following parts of this section continue to follow the error effect through the Prony fit for Case 2 with $r_1^2/\lambda^2 = 8.16 \times 10^{-10}$.

The second step in the Prony method is to calculate $\lambda_1$, $\lambda_2$, and $\lambda_3$ as the roots of the equation:

$$\lambda^3 - \lambda_1 \lambda^2 - \lambda_2 \lambda - \lambda_3 = 0 \quad (B.14)$$

The error in $\lambda$ caused by error in the $\lambda_k$'s is given by:

$$\delta \lambda = \frac{\lambda^2 \delta \lambda_1 + \lambda \delta \lambda_2 + \delta \lambda_3}{3 \lambda^2 - 2 \lambda_1 \lambda - \lambda_2} \quad (B.15)$$

for $\lambda$ real. In this equation $\lambda$ and $\lambda_k$ are the true values of these parameters and $\delta \lambda_k$ is the error in the calculated value of $\lambda_k$ due to the measurement error.

Expressions similar to (B.15) exist for calculating the error when $\lambda$'s exist as a pair of complex roots:

$$\lambda = \lambda_R \pm i \lambda_I \quad (B.16)$$

The case under consideration has a pair of complex roots $\lambda_R \pm i \lambda_I$ and one real root $\lambda_3$. From the known true values of $\lambda_R$, $\lambda_I$, $\lambda_3$, $\lambda_1$, $\lambda_2$, and $\lambda_3$ and the calculated errors $\delta \lambda_1$, $\delta \lambda_2$, and $\delta \lambda_3$, the errors in the $\lambda$'s are given by:

$$\delta \lambda_3 = -23.83408 \epsilon^2 \times 10^5$$
$$\delta \lambda_R = 1.8204 \epsilon^2 \times 10^3$$
$$\delta \lambda_I = 4.6812 \epsilon^2 \times 10^3 \quad (B.17)$$
Since \( \mu_3 = e^{r_3} \),

\[
\mathcal{S} r_3 = \frac{\mathcal{S} \mu_3}{e^{r_3}} = -26.60647 \in \mathbb{R} \times 10^5. \tag{B.19}
\]

Further, recall that the linear change of time variables was imposed such that \( x = t/\Delta t \) or \( t = x \Delta t \).

Then \( e^{r_3 x} = e^{a_3 t} \),

\[
ea_3 = \frac{r_3 x}{x \Delta t} = \frac{r_3}{\Delta t}. \tag{B.21}
\]

Then:

\[
\mathcal{S} a_3 = \frac{\mathcal{S} r_3}{\Delta t} = -354.75293 \in \mathbb{R} \times 10^5. \tag{B.22}
\]

For the complex roots:

\[
\ln (\mu_R + i \mu_I) = \ln u e^{i \theta} = \ln u + i \theta. \tag{B.23}
\]

where \( u = \sqrt{\mu_R^2 + \mu_I^2} \) and \( \theta = \tan^{-1} \frac{\mu_I}{\mu_R} \).

Then

\[
\mathcal{S} u = \frac{2 \mu_R \mathcal{S} \mu_R + 2 \mu_I \mathcal{S} \mu_I}{2r} = 5.00369 \in \mathbb{R} \times 10^3. \tag{B.25}
\]

Since \( u = e^r \),

\[
\mathcal{S} r = \frac{\mathcal{S} u}{e^r} = 12.43153 \in \mathbb{R} \times 10^3. \tag{B.27}
\]

and with the change of time variables:

\[
a = \frac{r}{\Delta t}, \tag{B.28}
\]

\[
\mathcal{S} a = \frac{\mathcal{S} r}{\Delta t} = 165.75373 \in \mathbb{R} \times 10^3. \tag{B.29}
\]
\[
\theta = \tan^{-1} \frac{\mu_I}{\mu_R}, \quad \text{(B.30)}
\]

\[
\delta \theta = \frac{\mu_R \delta \mu_I - \mu_I \delta \mu_R}{R^2 \sec^2 \theta} \quad \text{(B.31)}
\]

From the known true values for the case being examined:

\[
\delta \theta = -1.0856 \varepsilon^2 \times 10^3 \quad \text{(B.32)}
\]

For the change of time variables:

\[
b = \frac{\theta}{\Delta t} \quad \text{(B.33)}
\]

\[
\delta \theta = \frac{\delta \theta}{\Delta t} = -14.47467 \varepsilon^2 \times 10^3 \quad \text{(B.34)}
\]

The errors in the calculation of the \( \mu \)'s are of comparable magnitudes to the errors in the \( \delta \lambda \)'s. For this reason it is concluded that no appreciable error growth takes place in this section of the Prony fit.

The last step in the Prony method solves the system:

\[
C_0 + C_1 e^{r_k} \cos k \theta + C_2 e^{r_k} \sin k \theta + C_3 e^{r_3 k} = y_k, \quad k = 0, 1, \ldots, N-1 \quad \text{(B.35)}
\]

for the coefficients \( C_0, C_1, C_2, \) and \( C_3. \)

For the errors in the coefficients caused by the measurement error \( \varepsilon \) implicit in \( \delta r, \delta \theta, \) and \( \delta r_3: \)

\[
\delta C_0 + \delta C_1 e^{r_k} \cos k \theta + \delta C_2 e^{r_k} \sin k \theta + \delta C_3 e^{r_3 k} = \delta y_k + (C_1 \delta \theta - C_2 \delta r) ke^{r_k} \sin k \theta
\]

\[
- (C_1 \delta r + C_2 \delta \theta) ke^{r_k} \cos k \theta + C_3 \delta r_3 k e^{r_3 k},
\]

\[
= \delta Y_k, k, k = 0, 1, \ldots, N-1. \quad \text{(B.36)}
\]
The normalized $4 \times 4$ matrix of coefficients for (B.36) is equal to the normalized matrix of coefficients for (B.35), the error free equations. The corresponding $4 \times 1$ vector $\eta_j$ has elements:

$$\eta_j = \sum_{k=0}^{N-1} \xi_k h_{kj}, \ j = 1, 2, 3, 4$$  \hspace{1cm} (B.37)

where the $h_{kj}$ are the elements of the coefficient matrix of (B.35).

The errors in the coefficients can then be calculated from the normalized system in terms of the known true values and the calculated errors $\delta r, \delta \theta, \delta r_3$. Thus:

$$\delta c_0 = -25.87936 \times 10^{-3},$$
$$\delta c_1 = 106.1755 \times 10^{-3},$$
$$\delta c_2 = 188.784 \times 10^{-3},$$

and

$$\delta c_3 = -82.39276 \times 10^{-3}. \hspace{1cm} (B.38)$$

Again, since the magnitudes of these errors are of the same order as the errors $\delta r, \delta \theta, \delta r_3$, no error growth occurs in this section.

Referring to Equation (B.37) and substituting the true values of $c_1, c_2, c_3, r, \theta$, and $r_3$ and the calculated values of the errors $\delta c_0, \delta c_1, \delta c_2, \delta c_3, \delta r, \delta \theta$, and $\delta r_3$ gives:

$$\delta \Psi_k = 10^3 \xi^2 \left[ -25.89936 + 106.1755 e^{rk} \cos k\theta \\
+ 188.784 e^{rk} \sin k\theta - 82.39276 e^{r_3 k} \\
+ 26.11727 k e^{rk} \cos k\theta + 2.65214 k e^{rk} \sin k\theta \\
+ 24.3183 e^{r_3 k} \right]$$
\[ = 10^3 \epsilon^2 p_k, \ k = 0, 1, 2, \ldots, N - 1 \quad (B.39) \]

The value of \( \mathcal{S} y_k \) given by Equation (B.39) is the error occurring in the kth value of the step response calculated from the fitted equation. The error in the fitted equation is caused by the single error \( \epsilon \) in observing the ith value of the step response. For an error \( \pm \epsilon \) occurring at each of the N observed values of the step response the effect should be additive. The error in the kth calculated value of the step response caused by errors in all N of the observed values of the step response is:

\[ y_k = 10^3 N \epsilon^2 p_k, \ k = 0, 1, 2, \ldots, N-1 \quad (B.40) \]

If it is assumed that the squared error \( \epsilon^2 \) is equal to the mean square error:

\[ \epsilon^2 = \overline{r_i^2}, \quad (B.41) \]

then

\[ \mathcal{S} y_k = 10^3 N \overline{r_i^2} p_k. \quad (B.42) \]

The mean square value \( \mathcal{S} \overline{y^2} \) was calculated over \( k = 0, 1, 2, \ldots, N - 1 \) and found to be \( \mathcal{S} \overline{y^2} = 10.879 \times 10^{-6} \) which is slightly larger than the "effective" mean square error, \( \overline{r_i^2} = 4.0187 \times 10^{-6} \).

The large differences between the predicted and observed values of \( \mathcal{Y}_{LE} \) can thus be explained by error growth in the Prony fit of the observed data to the linear model. This error growth occurs in the least square solution of the N-4 equations given by (B.5) for \( \alpha_1, \alpha_2, \) and \( \alpha_3 \). The error
growth results from the small value of the determinant of the normalized coefficient matrix of Equation (B.12). It was found that as the ratio $\frac{f_1^2}{A^2}$ increases the value of this determinant increases, and the error growth decreases. Further evidence of this is exhibited in Table 9. Table 9 is a tabulation of $\frac{f_1^2}{A^2}$, $\frac{\overline{\gamma}_{\text{LE}}}{A^2}$ and the ratio $\frac{\overline{\gamma}_{\text{LE}}}{(f_1^2/A^2)}$ for Case 1. The ratio can be considered as a measure of the error growth in the Prony analysis. Observe that the ratio decreases as the value of $\frac{f_1^2}{A^2}$ increases. The error criterion $\frac{\overline{\gamma}_{\text{LE}}}{A^2}$ behaves in the expected manner and increases with $\frac{f_1^2}{A^2}$.

Since the error growth in the Prony method is the result of an ill-conditioned matrix, several possibilities exist for achieving a more accurate description of the step response in terms of Equation (B.3). This section presents two of these.

The first method consists of an iterative procedure for improving the accuracy of the inverse of the normalized matrix. If the set of N-4 equations in 3 unknowns implied by Equation (B.4) is:

$$Y_a = z,$$  \hspace{1cm} (B.43)

the 3 x 3 set of normalized equations is given by:

$$Y^TY_a = Y^Tz,$$  \hspace{1cm} (B.44)

$$Aa = c$$  \hspace{1cm} (B.45)

and

$$a = A^{-1}c$$  \hspace{1cm} (B.46)
Following the development in Lapidus\textsuperscript{8}, for B the approximate inverse of A and $B + \Delta B$ the exact inverse:

$$A \ (B + \Delta B) = I.$$  \hspace{1cm} \text{(B.47)}

Premultiplying by $B$ and re-arranging gives:

$$BA \ \Delta B = B \ (I - AB).$$  \hspace{1cm} \text{(B.48)}

But $BA \approx I$ so that an approximate relation is:

$$\Delta B = B \ (I - AB),$$  \hspace{1cm} \text{(B.49)}

$$B + \Delta B = B \ (2I - AB).$$  \hspace{1cm} \text{(B.50)}

The resulting iteration sequence is:

$$B^1 = B^0 \ (2I - AB^0)$$

$$B^2 = B^1 \ (2I - AB^1)$$

$$\vdots$$

$$B^{r+1} = B^r \ (2I - AB^r)$$  \hspace{1cm} \text{(B.51)}

$$\lim_{r \to \infty} B^{r+1} = A^{-1}$$  \hspace{1cm} \text{(B.52)}

The necessary and sufficient condition for (B.11) to converge is that the eigenvalues of $I - AB^0$ have moduli less than 1.0. This condition is achieved in practice when $B^0$ is a reasonable approximation to $A^{-1}$.

The second approach uses search techniques in an iterative solution of the set of $N$ equations in $7$ unknowns implied by Equation (B.4). For the observed data $y_k$ at discrete points of $t = k \Delta t$, $k = 0, 1, \ldots, N - 1$, it is
desired to evaluate the fit:

$$y_k' = c_0 + \sum_{i=1}^{3} c_i e^{a_i t},$$  \hspace{1cm} \text{(B.53)}

or

$$y_k' = c_0 + e^{at} (c_1 \cos bt + c_2 \sin bt) + c_3 e^{a_3 t}$$  \hspace{1cm} \text{(B.54)}

such that

$$M = S^2 = \sum_{k=0}^{N-1} (y_k' - y_k)^2 = \min.$$  \hspace{1cm} \text{(B.55)}

For this case there are 7 variables to be evaluated ($c_0$, $c_1$, $c_2$, $c_3$, $a_1$ or $a$, $a_2$ or $b$, $a_3$). The C's are not independent since for $t = 0$,

$$c_0 + c_1 + c_2 + c_3 = y_0$$  \hspace{1cm} \text{(B.56)}

or

$$c_0 = y_0 - c_1 - c_2 - c_3.$$  \hspace{1cm} \text{(B.57)}

Define the dimensionless vector $x$ by scaling the six remaining variables over their probable span:

$$x = \left( \frac{c_i - c_{i \text{ min}}}{c_{i \text{ max}} - c_{i \text{ min}}} 10, \frac{c_i - c_{i \text{ min}}}{c_{i \text{ max}} - c_{i \text{ min}}} 10, \ldots, \right.$$  \hspace{1cm} \text{(B.58)}

$$\left. \frac{a_3 - a_{3 \text{ min}}}{a_{3 \text{ max}} - a_{3 \text{ min}}} 10 \right).$$

such that $0 \leq x \leq 10$.

An experiment to determine the gradient at the point $x_n$ consists of taking observations at $x_n$ and at 6 other points which differ from $x_n$ in that exactly one of their 6
coordinates has been increased by the small constant
distance $c$. Let $e_j$ be the $j$th unit vector whose $j$th element
is one and the rest zero. The $n$th block of experiments is
then defined by observations at the following 7 points:

\[
x_n^0 = x_n \\
x_n^1 = x_n + ce_1 \\
x_n^2 = x_n + ce_2 \\
\vdots \\
x_n^6 = x_n + ce_6
\]  
\[(B.59)\]

Let $M_n^j$ be the value of the objective function calcu-
lated for the point $x_n^j$, so that:

\[
M_n^j = M( x_n^j ), \quad j = 1, 2, \ldots, 6. \quad (B.60)
\]

The normalized version of the gradient at $x_n$ is then defined
as the vector $m$ whose $j$ component is:

\[
m_n^j = \text{sgn} \left( \frac{M_n^j - M_n}{c} \right) = \frac{(M_n^j - M_n)}{|M_n^j - M_n|} \quad (B.61)
\]

The next base point $x_{n+1}$ is placed in the opposite
direction from that given by this estimated gradient, i.e.,

\[
x_{n+1} = x_n - a_n m, \quad (B.62)
\]

where the step size $a_n$ is the harmonic sequence $1, \frac{1}{2}, 1/3, \ldots$
Following the acceleration procedure based on Kesten's
modification of the Kiefer-Wolfowitz procedure\textsuperscript{10}, no
experiment is performed at \( x_{n+1} \) unless

\[
M_{n+1} - M_n > 0. \quad (B.63)
\]

Furthermore, the search continues in the direction given by \(-m\), taking steps of magnitude \( a_n \), until the above condition is fulfilled. Only then is another experiment performed and the step size \( a_n \) advanced to the next value in the harmonic sequence. Thus, the step size shortens only when the approach to the minimum is signaled by sign oscillation.

The procedure converges with probability one for:

\[
a_{n+1} < a_n \text{ for all } n = 1, 2, 3 \ldots \quad (B.64)
\]

and

\[
c_n = \text{ constant for all } n = 1, 2, 3 \ldots \quad (B.65)
\]

The first condition is satisfied by the harmonic sequence. The rate of convergence depends on the choice made in scaling the independent variables.

The starting values for the search could be supplied by the values of \((C_0, C_1, C_2, C_3, a_1 \text{ or } a, a_2 \text{ or } b, a_3)\) obtained from the Prony fit or from completely arbitrary values. In either case the method is confounded by the choice of the form of the solution to fit and encumbered by a large number of calculations.
BIBLIOGRAPHY


