AN IMPROVED METHOD FOR PROCESS IDENTIFICATION IN THE FREQUENCY DOMAIN

C. H. Tu and J. N. Petersen
Department of Chemical Engineering, Washington State University, Pullman, WA 99164, U.S.A.

(Received 11 November 1981; in revised form 3 May 1982; received for publication 15 June 1982)

Abstract - An improved method which used frequency domain data for the determination of process transfer functions is presented. The method presented uses a sign transformation for regression models to ensure positive parameters. A statistical test, based on a right-hand tail F-ratio test and an uncertainty test, is discussed for selecting an adequate system transfer function. The procedure is demonstrated by two examples.

Frequency domain Process identification Transfer function Dead time

INTRODUCTION

With increasing frequency, biomedical researchers are using transfer functions to describe linear systems [1-4]. One of the most important advantages of transfer functions is the ease with which processes can be analyzed in any of a variety of manners. However, in many situations, transfer functions cannot be written from a theoretical knowledge of the system. For these reasons, identification of the transfer function from experimental data is a useful activity.

Recently, two well-developed experimental methods have been proposed for the determination of process transfer functions. One method uses time-domain determination [5] and the other uses frequency-domain determination [6-13]. For many problems, however, it is much simpler and computationally advantageous to evaluate the model in the frequency domain [7, 11, 14].

The general approach begins by applying an experimental test to the process under study. Among the experimental techniques, sine-wave testing, step testing and pulse testing are the ones most widely used. Previous workers [6-9] have favored using pulse tests because the test is simple to generate and has a short test time. The pulse test results in two continuous curves of input and response recorded as functions of time. In the usual method for analyzing the response from a pulse test, dead time determination presents a problem. If any dead time exists in the system, the dead time is usually read from the continuous curves by observing when the first deviation from the steady state occurs. This time is assumed to be the dead time of the process. Also, any dead time should be removed from the test data by changing the zero-time of the response signal to the point of the first observable deviation in this signal [11]. The technique presented here does not require these assumptions concerning dead time.

To apply the technique, a reasonable number of points must be selected from the records and fed into a digital computer. The computer then evaluates the Fourier transform of the data and outputs the frequency response data. This information includes an amplitude ratio and a phase angle at each frequency. In addition, the steady state gain of the process is obtained from the Fourier transform. Once these data have been obtained, they are correlated into a proper transfer function.

This correlation process assumes that the process can be represented by either a first-, a second-, or a third-order transfer function [7-11]. A non-linear regression technique is then applied directly to the amplitude ratio form of these data [7, 11]. Finally a statistical test is used in selecting an adequate representation for the process [11].

The above general scheme, however, fails to incorporate the important phase angle information within the model and is unable to account for the parameter sign restriction in
the model. Moreover, no statistical criteria are used to indicate which transfer function form is most appropriate.

By noting that the parameters in the transfer function must be non-negative for realistic systems, this work presents a sign transformation for regression models to ensure positive parameters. A proper statistical test, based on a right-hand tail F-ratio test and an uncertainty test, is used for selecting an adequate system transfer function. Instead of reading dead time from the results of the experimental tests, a dead time determination procedure is developed. With these improvements, the method presented here can be expected to be utilized in an on-line fashion for system analysis.

**FORMULATION OF THE METHOD**

**Calculation of \( G(j\omega) \) from pulse test data**

Consider a process as shown in Fig. 1. This process may represent any system from a complex chemical plant to the response of a nerve when stimulated.

By definition, the transfer function of the process is

\[
G(s) = \frac{Y(s)}{X(s)} = \frac{Y(t)}{X(t)}
\]

where \( s \) = Laplace transfer variable with respect to time, \( t \); \( X(s) \) = Laplace transform of input, \( X(t) \), in deviation form; and \( Y(s) \) = Laplace transform of output, \( Y(t) \), in deviation form.

Using the definition of the Laplace transform

\[
G(s) = \frac{\int_{0}^{\infty} Y(t)\exp(-st)\,dt}{\int_{0}^{\infty} X(t)\exp(-st)\,dt}
\]

it is possible to go into the frequency domain by substituting \( s = j\omega \) where \( j = \sqrt{-1} \) and \( \omega \) represents frequency.

\[
G(j\omega) = \frac{\int_{0}^{\infty} Y(t)\exp(-j\omega t)\,dt}{\int_{0}^{\infty} X(t)\exp(-j\omega t)\,dt}
\]

The numerator is the Fourier transform of the time function \( Y(t) \). The denominator is the Fourier transform of the time function \( X(t) \). Several techniques are available for evaluating the Fourier transform of a series of data. Among these are the fast Fourier transform (FFT) [15]. An excellent text by Bracewell [16] discusses the many aspects of the Fourier transform. It is not the purpose of this paper to discuss this information.

**Theoretical considerations for the identification of dynamic processes**

For the identification, it was assumed that any process could be represented by either a first-, second-, or a third-order linear ordinary differential equation (ODE). When linear ODEs describing a system are Laplace transformed, they yield first-, second-, and third-order transfer functions.

For a general first-order system

\[
G_1(s) = \frac{K}{TS + 1} \exp(-DS).
\]

Fig. 1. Block diagram of a process.
An improved method for process identification in the frequency domain

For a general second-order system,

\[ G_2(s) = \frac{K}{T^2s^2 + 2\zeta Ts + 1} \exp(-DS). \]  

(5)

For a general third-order system,

\[ G_3(s) = \frac{K}{(T_1s + 1)(T_2s^2 + 2\zeta Ts + 1)} \exp(-DS) \]  

(6)

where \( T, T_1 \) = system time constants; \( K \) = system steady state gain; \( D \) = dead time or transportation lag; and \( \zeta \) = damping coefficient.

In order to correlate the frequency-response data, the above transfer function forms must be expressed in terms of the amplitude ratio and the phase angle. As an example, for the second-order transfer function,

\[ \text{mag } G_2 = K\left[\left(1 - T^2 \omega^2\right)^{1/2} + \phi\beta \right] \]  

and

\[ \text{arg } G_2 = \arctan \left( \frac{-2\zeta T \omega}{1 - T^2 \omega^2} \right) - D\omega. \]  

(7a)

(7b)

To ensure non-negative time constants, damping coefficient and dead time, several transformations can be considered [17]. The transformation by absolute expression is the most suitable in this case. With the reparameterized absolute expressions for the sign constraint, these forms are now written as

\[ \text{mag } G_2 = K\left[\left(1 - |\theta|\omega^2\right)^{1/2} + |\phi|\omega^2\right]^{1/2} \]  

and

\[ \text{arg } G_2 = \arctan \left( \frac{-|\phi|\omega}{1 - |\theta|^2 \omega^2} \right) - |x|\omega \]  

(8)

(9)

where \( |\theta| = T; |\phi| = 2\zeta T; \) and \( |x| = D. \)

\[ \text{mag } G_2 = \text{the second-order amplitude ratio form} \]

\[ \text{arg } G_2 = \text{the second-order phase angle form}. \]

It is necessary to use a non-linear regression technique for the parameter regression. Several well-developed algorithms are available. Among these are a modified Taylor series method [11], a maximum neighborhood method [18] and a transformational discrimination method [19]. Again, it is not the purpose of this paper to discuss this information.

Criteria for an appropriate representation

Before describing what criteria were used to choose the most adequate representation, it is necessary to define certain fundamental concepts.

(1) Number of degrees of freedom, \((n - p)\). In statistical terminology the number of degrees of freedom is defined as the number of data points \(n\) minus the number of unknown parameters \(p\). This quantity allows for a mathematical correction of the data for constraints placed on the data. If a total of \(n\) data points are used to evaluate \(p\) unknown parameters, then \(p\) constraints have been placed on the data.

(2) Residuals. The differences between the observed and the calculated variables are called the residuals of these variables.

(3) The sum of the squares of the residuals. The sum of the squares of the residuals \((S^2)\) is the summation of the squared residuals of a certain number of the data points.

(4) Standard error of estimate. The standard error of estimate \((SE)\) is defined as the square root of the average minimized sum of the squares of the residuals.

In order to simplify the selecting criteria, the frequency response data are regarded as error free if compared to the three transfer functional forms. That is, it is assumed that any errors in
the data are meaningless when compared to the errors deriving from the failure of a true functional form to fit the data. These are called errors due to lack of fit [11]. It is also assumed that the uncertainties in the values of frequency are negligibly small if compared to the uncertainties in the values of amplitude ratio and phase angle data.

The method of least squares was used to determine the value of the parameters which minimize the sum of the squares of the residuals of the dependent variables. This minimized sum of the squares is a measure of the errors due to lack of fit.

Since all minimized sums of the squares of the residuals, $S_2^2$, were calculated from the same number of data points and using the same procedure of the non-linear regression technique, the ratios between each two sums could be expected to form some type of frequency distribution. This distribution can be expected to depend on the number of degrees of freedom used in estimating $S_2^2$. The values of these distributions would then depend on the respective degrees of freedom. These particular distributions have been mathematically derived and tabulated [19]. For example, they can be denoted as $F(v_1, v_2) = S_1^2/S_2^2$ distributions, where $v_1$ and $v_2$ are the degrees of freedom referred to $S_1^2$ and $S_2^2$ respectively.

Now assume that when the non-linear regression is applied to the transfer functional forms, the result which gives the smallest value of $S_2^2$ is always significant in predicting the system. Evaluating the $F$-ratio defined here provides a measure of significance for the regression on the other transfer functional forms when compared with the one with the smallest value of $S^2$.

That is, evaluating the $F$-ratio gives a test of the significance of estimated errors due to lack of fit. Errors due to lack of fit are, of course, assumed to be distributed with mean zero and variance $\sigma^2$.

The $F$-ratio can be computed from

$$ F = \frac{\text{larger } S^2}{\text{smaller } S^2} $$

$H_0(\sigma_1^2 = \sigma_2^2)$ is then tested against $H_0(\sigma_1^2 \neq \sigma_2^2)$. If $S_1^2$ is larger than $S_2^2$ and tests at a significance level $\alpha$, $H_0$ can be accepted when $F(v_1, v_2) \leq F_{\alpha, 2}(v_1, v_2)$. If $S_1^2$ is smaller than $S_2^2$, $H_0$ can be accepted when $F(v_2, v_1) \leq F_{\alpha, 2}(v_2, v_1)$. If $H_0$ is accepted, the prediction with the larger $S^2$ is also significant. If $H_0$ is rejected, the prediction with the larger $S^2$ should be laid aside.

The standard error of estimate is a direct measure of scatter and thus the goodness-of-fit, of the regression equation [22]. If the $F$-test is passed, the standard errors of estimate are compared in order to choose an appropriate representation for the process. The one with the smallest standard error of estimate is chosen as the best representation.

Based on the above considerations, the following criteria can be used to select an appropriate representation.

Let $z$ = the significance level of the test, $F_z$ = the $F$-distribution at significance level of $z$, and $n$ = the number of data points.

If $S_1^2$ is the smallest, there are two cases as follows.

**Case I.** $S_3^2 < S_2^2 < S_1^2$.

- If $(S_2^2/S_1^2) > F_{x/2}(n - 2, n - 1)$, use the first-order.
- If $(S_2^2/S_1^2) \leq F_{x/2}(n - 2, n - 1)$, make the following test.
- If $(S_2^2/S_3^2) \leq F_{x/2}(n - 3, n - 1)$, make the following test.

Compare $SE_1$, $SE_2$, and $SE_3$. The order with the smallest value is the best.

- If $(S_2^2/S_3^2) > F_{x/2}(n - 3, n - 1)$, make the following test.
- Compare $SE_1$ and $SE_2$. The order with the smaller value is better.

**Case II.** $S_1^2 < S_3^2 < S_2^2$.

- If $(S_2^2/S_3^2) > F_{x/2}(n - 3, n - 1)$, use the first-order.
- If $(S_2^2/S_3^2) \leq F_{x/2}(n - 3, n - 1)$, make the following test.
- If $(S_2^2/S_1^2) \leq F_{x/2}(n - 2, n - 1)$, make the following test.

Compare $SE_1$, $SE_2$, and $SE_3$. The order with the smallest value is the best.

- If $(S_2^2/S_3^2) > F_{x/2}(n - 2, n - 1)$, make the following test.
- Compare $SE_1$ and $SE_3$. The order with the smaller value is better. The above procedure gives only the example of $S_1^2$ being the smallest. The other conditions, $S_2^2$ and $S_3^2$ being the smallest, should be similarly treated for the complete criteria.
An improved method for process identification in the frequency domain

**Dead-time determination**

Once the amplitude ratio data have been properly fitted by an approximate transfer function, the dead time must be determined to complete the model. When the phase angles of this approximate transfer function are compared with the experimental phase angles, the differences are considered due to dead time.

The time delay (dead time) differs from the time lag in that it holds signals back in time instead of merely weakening them. A simple but common example is the dead time which arises when the measuring point of some process variable resides downstream from the actual point of interest.

The transfer function of a dead time is \( \exp(-Ds) \). The frequency-response characteristics are found in the usual way by substituting \( j\omega \) for \( s \) in the transfer function. Since, by Euler's formula, \( \exp(-j\omega D) = \cos(\omega D) - j \sin(\omega D) \), the amplitude ratio, given by the square root of the sum of the squares of the real and imaginary parts, is equal to 1.0. The phase angle, given by the arctangent of the ratio of the imaginary part to the real part, is equal to \(-\omega D\). If the dead time is included in a transfer function, it decreases the phase angle of the transfer function by \( D\omega \) but has no effect on the amplitude ratio.

The same non-linear regression technique is used to determine a reasonable dead time for the model. The procedure for determining dead time can be summarized as follows:

1. Collect a reasonable number of experimental data points.
2. Calculate the theoretical phase angles at corresponding frequencies from the approximate transfer function selected by performing the statistical test described above on the amplitude-ratio data.
3. Obtain the differences between the phase angles calculated from the theoretical transfer function and the experimentally determined phase angles.
4. Use the same regression technique as is used in the above tests to determine the dead time \( D \).

**APPLICATIONS AND DISCUSSION**

Two applications illustrating the method developed above are presented. The method was tested by arriving at an appropriate transfer function representation from Bode data.

In order to test the method, it was necessary to create simulated experimental Bode data from known transfer functions. A reasonable number of true amplitude ratio data were chosen and randomized by a uniform random number generator. These randomized amplitude ratio data, together with the phase angle data, were then used to evaluate the technique presented above.

**Application 1**

In the first system used to test the method, the transfer function

\[
G(s) = \frac{1}{s + 1} \exp(-0.05s)
\]

was selected. This first-order system was used to generate Bode data. The amplitude ratio data listed in Table 1 were taken from the true data after being randomized multiplicatively from 0.9 to 1.1. That is, \( R_A_i = T_A_i \times V_i \) where

- \( R_A_i \) = the randomized value of the \( i \)th point,
- \( T_A_i \) = the true value of the \( i \)th point, and
- \( V_i \) = a random number between 0.9 and 1.1.

The nonlinear regression technique on the three amplitude ratio forms gave the following results.

First order without dead time:

\[
G_1(s) = \frac{1}{(0.9512s + 1)}
\]
Table 1. Bode data from the first-order system (Application 1).

<table>
<thead>
<tr>
<th>Frequency (rad/time)</th>
<th>Amplitude ratio</th>
<th>Phase angle (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000</td>
<td>0.7235</td>
<td>-47.8647</td>
</tr>
<tr>
<td>1.995</td>
<td>0.4822</td>
<td>-69.0964</td>
</tr>
<tr>
<td>3.162</td>
<td>0.3139</td>
<td>-81.5107</td>
</tr>
<tr>
<td>3.981</td>
<td>0.2440</td>
<td>-93.074</td>
</tr>
<tr>
<td>5.012</td>
<td>0.1916</td>
<td>-112.9371</td>
</tr>
<tr>
<td>6.310</td>
<td>0.1658</td>
<td>-112.9371</td>
</tr>
<tr>
<td>10.000</td>
<td>0.11723</td>
<td>-112.9371</td>
</tr>
</tbody>
</table>

$S_1^2$ (sum of the squares of the residuals) = 0.002784
SE$_1$ (standard error of estimate) = 0.01918.

Second order without dead time:

\[
G_2(S) = \frac{1}{(0.0553 S^2 + 0.9940S + 1)}
\]

\[S_2^2 = 0.002622\]
\[SE_2 = 0.02090\]

Third order without dead time:

\[
G_3(S) = \frac{1}{(0.0113S + 1)(0.1977S^2 + 1.169S + 1)}
\]

\[S_3^2 = 0.01796\]
\[SE_3 = 0.5944\]

The statistical test to choose an appropriate representation was applied by first using the right-hand tail $F$-test with a significance level of 0.10.

\[
S_1^2/S_2^2 = 1.048 < F_{0.05}(7,6) = 4.21
\]
\[
S_3^2/S_2^2 = 6.850 > F_{0.05}(5,6) = 4.39.
\]

Since the first ratio of the sums of the squares of the residuals was well within the corresponding $F$ value, the regression on the first-order representation was also significant. The regression on the third-order was, however, insignificant because the second ratio of the sum of the squares of the residuals exceeded the corresponding $F$ value. Thus, there were two representations which were acceptable for the system. When the estimated standard errors of these two orders were compared,

\[SE_1 = 0.01981 < SE_2 = 0.02090;\]

the result favored the first order representation. Finally, by using the strategy of noting the influence of dead time on the phase angle, the system dead time was found to be 0.05158 unit time.

Therefore, the transfer function which best represented the system was the first order with

\[
G(S) = \frac{1}{(0.9512S + 1)} \exp(-0.05158S).
\]

The parameters with 90% confidence limits can be expressed as 0.9512 ± 0.0642 and 0.05158 ± 0.00368. The resulting Bode plot is shown in Fig. 2.

Application 2

This application was also used to test the method by obtaining a proper system transfer
function from Bode data. The known transfer function, a third-order system, was used to generate true Bode data. This actual function is given by

\[ G(S) = \frac{1}{(S + 1)(S^2 + 0.6S + 1)} \exp(-0.4S). \]  

(15)

The amplitude ratio data in Table 2 were taken from the true data after being randomized multiplicatively from 0.9 to 1.1.

Use of the non-linear regression technique on the three amplitude ratio forms gave the following results.

First order without dead time:

\[ G_1(S) = \frac{1}{0.8634S + 1} \]  

(16)

\[ S_1^2 = 0.9662 \]

\[ SE_1 = 0.2726. \]

<table>
<thead>
<tr>
<th>Table 2. Bode data from the third-order system (Application 2).</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Frequency (rad/time)</th>
<th>Amplitude ratio</th>
<th>Phase angle (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>1.0465</td>
<td>-3.1459</td>
</tr>
<tr>
<td>0.100</td>
<td>1.0103</td>
<td>-11.4706</td>
</tr>
<tr>
<td>0.200</td>
<td>1.0371</td>
<td></td>
</tr>
<tr>
<td>0.316</td>
<td>1.1156</td>
<td>-11.4706</td>
</tr>
<tr>
<td>0.398</td>
<td>1.1130</td>
<td>-59.9854</td>
</tr>
<tr>
<td>0.501</td>
<td>1.0988</td>
<td>-11.4706</td>
</tr>
<tr>
<td>0.631</td>
<td>1.1647</td>
<td>-59.9854</td>
</tr>
<tr>
<td>0.794</td>
<td>1.3766</td>
<td>-11.4706</td>
</tr>
<tr>
<td>1.000</td>
<td>1.1142</td>
<td>-157.9186</td>
</tr>
<tr>
<td>1.259</td>
<td>0.0807</td>
<td>-157.9186</td>
</tr>
<tr>
<td>1.995</td>
<td>0.1256</td>
<td>-267.2275</td>
</tr>
<tr>
<td>3.162</td>
<td>0.0324</td>
<td>-313.0183</td>
</tr>
<tr>
<td>3.981</td>
<td>0.0167</td>
<td>-337.9992</td>
</tr>
<tr>
<td>5.012</td>
<td>0.0088</td>
<td>-366.4695</td>
</tr>
</tbody>
</table>
Second order without dead time:

\[ G_2(S) = \frac{1}{(1.2028S^2 + 0.9214S + 1)} \]  
\[ S^2_2 = 0.05615 \]
\[ SE_2 = 0.06840. \]

Third order without dead time:

\[ G_3(S) = \frac{1}{(0.9644S + 1)(1.0786S^2 + 0.6308S + 1)} \]  
\[ S^2_3 = 0.01534 \]
\[ SE_3 = 0.03735. \]

Upon applying the F-test with a significance level of 0.10,

\[ S^2_2/S^2_3 = 3.66 > F_{0.05}(12,11) = 2.72 \]
\[ S^2_2/S^2_3 = 62.98 > F_{0.05}(13,11) = 2.76. \]

Since both ratios of the sums of the squares of the residuals exceeded the corresponding F values, neither the first-order nor the second-order transfer function was valid. Thus, the proper representation was the third-order. By the dead-time determination procedure, the system dead time was determined to be 0.3987 unit time. The approximate system transfer function was third-order with

\[ G(S) = \frac{1}{(0.9644S + 1)(1.0786S^2 + 0.6308S + 1)} \exp(-0.3987S). \]  

The parameters with 90% confidence intervals are 0.9644 ± 0.2704, 1.0786 ± 0.0701, 0.6308 ± 0.1075, and 0.3987 ± 0.0126. The resulting Bode plot is shown in Fig. 3.
SUMMARY

The scheme used in arriving at an appropriate process transfer function can be summarized as the following steps:

1. Obtain the frequency-response data of the system from experimental tests.
2. Assume that the system can be represented by a first-, second-, or a third-order transfer function.
3. Curve fit the amplitude ratio data to each of the three amplitude ratio forms with parameter sign constraints for the transfer functions.
4. Perform the statistical test to choose a proper representation of the process.
5. Determine any dead time in the process from the phase angle data.

As cited earlier, the pulse test was favored by previous investigators. The transfer functions proposed should be able to provide the system with adequate information in any circumstance. It is proper to incorporate the parameter sign transformation for both linear and nonlinear regression into the transfer functional forms.

The statistical test which is based on the F-ratio test and the standard error of estimate led to an appropriate system transfer function. Because phase angle decreases linearly with dead-time, it was possible to use a linear regression to determine the dead-time. Thus, the phase angle information could be included within the transfer function. The randomized frequency response data from two known systems verified that the improved method presented here is a powerful tool in the identification of dynamic processes.

REFERENCES


About the Author—CHUN-HUAN TU was born in Taiwan, Republic of China on April 14, 1951. He entered the Tatung Institute of Technology in 1970 and received a B.S. degree in chemical engineering in 1974. After two years' military service, he worked as a production engineer at Chang-Tai Chemical Industries Corporation, Kaoshuing Caprolactam Plant in Taiwan from 1976 to 1978. He then attended Washington State University where he obtained an M.S. degree in chemical engineering in 1981. His research interests are in mathematical modeling and process design and control.
About the Author — JAMES N. PETERSIN was born in Great Falls, Montana on 26 July 1954. He received his B.S. degree in chemical engineering at Montana State University in 1976 and his Ph.D. in chemical engineering (biomedical engineering) at Iowa State University in 1979. He has worked for Weyerhaeuser Co., Tacoma, WA and Chevron Research Co., Richmond, CA and is currently an Assistant Professor of Chemical Engineering at Washington State University. His research interests are in real time computer simulation, digital control and transport phenomena in living systems.