The Frequency Domain Evaluation of Mathematical Models for Dynamic Systems

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An important problem in the mathematical modeling of dynamic systems is the testing of model applicability and the determination of the best model parameters through the minimization of the squared difference of the observed and predicted responses. This paper discusses the advantages of the transformation of the expression for the integral of the squared deviations ϕ to the frequency domain by the use of Parseval's theorem. Two important advantages of the minimization of ϕ in the frequency domain are the ease with which the transform of the predicted response can be obtained and the algebraic nature of frequency domain operations. Other advantages are discussed and techniques for the numerical transformation and inversion of the observed and predicted responses are given.

The utility of mathematical models of chemical processes is often limited by their complexity. Since exact analytical solutions to many important differential equations are unobtainable, tedious numerical calculations are often required for the comparison of theoretical prediction with observation. In the field of control system analysis, this difficulty has been circumvented by the employment of approximate models of physical system dynamics. Model parameters are estimated by sinusoidal or pulse testing techniques (*4, 9, 10*) which require only the Fourier transform of the differential equation approximating the system and not the time domain solution. The model parameters are altered systematically until the magnitude ratios of the observed and predicted outputs match. This procedure usually neglects the effect of phase angle. The matching of observation and prediction in the frequency domain by this method ensures only approximate matching in the time domain.

Pulse testing techniques have also been used as the basis for the determination of important design parameters in a variety of distributed parameter flow systems. In particular, dispersivity has been calculated from tracer curves by the method of moments (*1, 2, 13*). Model parameters are estimated by matching the various moments of the data with corresponding moments predicted by the model. This method is disadvantageous for at least two important reasons. First, numerical errors associated with the computation of moments from experimental data can be quite large. Moment calculations weight heavily the "tail" portion of experimental time response curves, where measured curves are the least accurate. The weighting of the tail increases greatly as the order of the moment increases. Second, the moments method assumes in advance that the model is an excellent fit to the data; therefore no statistical information concerning the quality of the model fit is obtained from the fitting process. If the model happens to fit the data poorly, the parameters obtained will most likely be misleading and useless. It does not appear that moment methods will find general application in dynamic process modeling, except in those cases where the fit of the model to the data is known ahead of time to be quite good, and where the model incorporates only a few parameters so that use of the higher moments becomes unnecessary.

This paper presents a technique that uses both the real and imaginary parts of a system dynamic response to evaluate design and dynamic response parameters in linear lumped and distributed parameter systems. Parseval's theorem is used to formulate a Fourier transform domain comparison of the observed and predicted responses that is exactly equivalent to comparison of the time domain responses.

THE LEAST SQUARES CRITERION

Although many comparison criteria have been used in particular mathematical modeling applications, one of the simplest and most widely applicable criteria for dynamic systems is the integral of the squared error between the observed and predicted results. The integral should be formulated over all space and time but, for many applications, interest is directed to a particular point in space and the time varying error at this point is considered. Thus, the expression for the integral squared error at such a point is

$$\phi = \int_0^\infty [y_o(t) - y_p(t)]^2 \, dt \tag{1}$$

where $y_o(t)$ and $y_p(t)$ are, respectively, the observed and predicted responses.

Minimization of ϕ is commonly called the least squares procedure. Since the equations for the predicted response are in general nonlinear in the system parameters, an explicit least squares solution is usually not readily available, and the minimization of ϕ must be accomplished by a regression technique. Marquardt (*11, 12*) has developed an effective nonlinear least squares algorithm and has successfully incorporated it into a digital computer program.

For certain simple models it may be satisfactory to apply a nonlinear least squares procedure directly to the expression for ϕ given by Equation (1). However, for more complicated models, or for systems that have been excited by a measured input, it may be difficult to find and compute the predicted response $y_p(t)$. The following sections show how this can be avoided by transformation of the least squares criterion to the frequency domain.

FOURIER TRANSFORMATION

Restricted Definition

If $f(t)$ is a real function of time which is zero for all $t < 0$, then its associated Fourier transform pair (*5*) is

$$F(j\omega) = \int_0^\infty f(t)\, e^{-j\omega t}\, dt, f(t) = 0, t < 0 \quad (2)$$

$$f(t) = \frac{1}{\pi} \int_0^\infty F(j\omega)\, e^{j\omega t}\, d\omega, f(t) = \text{real} \quad (3)$$

Transformation of the Least Squares Criterion to the Frequency Domain

According to Parseval's theorem (*5*) there is a relationship between the squared magnitudes of the Fourier transform pair:

$$\int_0^\infty [f(t)]^2\, dt = \frac{1}{\pi} \int_0^\infty |F(j\omega)|^2\, d\omega \quad (4)$$

Application of this result to the least squares criterion given by Equation (1) yields the frequency domain expression for ϕ:

$$\phi = \frac{1}{\pi} \int_0^\infty |Y_o(j\omega) - Y_p(j\omega)|^2\, d\omega \quad (5)$$

Separation of Equation (5) into real and imaginary parts leads to the expression

$$\phi = \frac{1}{\pi} \int_0^\infty \{[R_o(\omega) - R_p(\omega)]^2 + [I_o(\omega) - I_p(\omega)]^2\}\, d\omega \quad (6)$$

It is now clear that while ϕ depends upon the squared scalar deviations in the time domain, it depends upon the squared vectorial deviations in the frequency domain.

It may be argued that the frequency domain modeling procedure should reflect a desire to minimize the deviations between the observed and predicted transfer functions as opposed to minimization of response deviations. It can be shown that if the transfer function deviations are weighted according to their experimental reliability, both points of view are equivalent. If $X(j\omega)$ represents the Fourier transform of the input function, Equation (5) can be rewritten as

$$\phi = \frac{1}{\pi} \int_0^\infty [|X(j\omega)|\, |Y_o(j\omega)/X(j\omega) - Y_p(j\omega)/X(j\omega)|]^2\, d\omega \quad (7)$$

The observed and predicted transfer functions are given, respectively, by the following equations.

$$G_o(j\omega) = Y_o(j\omega)/X(j\omega) \quad (8)$$

$$G_p(j\omega) = Y_p(j\omega)/X(j\omega) \quad (9)$$

Thus

$$\phi = \frac{1}{\pi} \int_0^\infty [|X(j\omega)|\, |G_o(j\omega) - G_p(j\omega)|]^2\, d\omega \quad (10)$$

The magnitude of the Fourier transform of the input pulse $|X(j\omega)|$ is a measure of the frequency content of the input pulse. It is an indication of the relative degree to which the system was excited at each frequency and can be interpreted as a weighting function measuring the relative reliability of the deviations at each frequency.

Numerical Fourier Transformation

The system response $y_o(t)$ is measured experimentally in the time domain, and it is necessary to have a method to transform $y_o(t)$ to $Y_o(j\omega)$ numerically in order to use Equation (6). The problem of finding the numerical Fourier transform of a function $f(t)$ that is given as a graph or a series of discrete points has been explored by Clements and Schnelle (*4*). Their approach in evaluating $F(j\omega)$ was to break the integral, given by Equation (2), into a real and an imaginary part as shown below:

$$F(j\omega) = \int_0^\infty f(t) \cos \omega t\, dt - j \int_0^\infty f(t) \sin \omega t\, dt \quad (11)$$

or

$$F(j\omega) = R(\omega) + j I(\omega) \quad (12)$$

The integrals representing $R(\omega)$ and $I(\omega)$ were evaluated with special quadrature formulas. However, the following method is more flexible and more efficient.

The method assumes that $f(t)$ can be represented by a function made up of a series of polynomial segments. Ordinary discontinuities in the function and its derivatives are allowed at the union of the segments. The time domain equation for this function is

$$f(t) \sim \sum_{i=1}^{n} u(t - T_i)\, [A_i + B_i(t - T_i) + C_i(t - T_i)^2 + D_i(t - T_i)^3 + \ldots] \quad (13)$$

where the change in the function over the interval T_{i-1} to T_i is given by A_i, the change over the interval in the first derivative at T_i is B_i, the change in the second derivative at T_i is C_i, etc. The notation $u(t - T_i)$ represents a unit step function and it indicates that additions to the function $f(t)$, causing the jumps at T_i, occur at time T_i. This expression is quite flexible and the approximating function can be made as simple or as complex as desired for any individual case. It includes as special cases, stepwise, linear and parabolic approximations to $f(t)$.

The Laplace transformation of Equation (13) is

$$F(s) \sim \sum_{i=1}^{n} \left[\frac{A_i}{s} + \frac{B_i}{s^2} + \frac{2C_i}{s^3} + \frac{6D_i}{s^4} + \ldots \right] e^{-T_i s} \quad (14)$$

If the function $f(t)$ is Fourier transformable, $j\omega$ can be substituted for s to give the Fourier transform.

$$F(j\omega) \sim \sum_{i=1}^{n} \left[\frac{A_i}{j\omega} + \frac{B_i}{-\omega^2} + \frac{2C_i}{-j\omega^3} + \frac{6D_i}{\omega^4} + \ldots \right] e^{-j\omega T_i} \quad (15)$$

Now $F(j\omega)$ can be written in terms of its real and imaginary parts as

$$R(\omega) \sim \sum_{i=1}^{n} \left[-\frac{A_i}{\omega} + \frac{2C_i}{\omega^3} - \ldots \right] \sin \omega T_i + \left[-\frac{B_i}{\omega^2} + \frac{6D_i}{\omega^4} - \ldots \right] \cos \omega T_i \quad (16)$$

$$I(\omega) \sim \sum_{i=1}^{n} \left[-\frac{A_i}{\omega} + \frac{2C_i}{\omega^2} - \ldots \right] \cos \omega T_i - \left[-\frac{B_i}{\omega^2} + \frac{6D_i}{\omega^4} - \ldots \right] \sin \omega T_i \quad (17)$$

Numerical Fourier Inversion

The symmetry of the Fourier transform pair makes possible the use of Equations (16) and (17) for inverse numerical Fourier transformation as well as for evaluation of the direct Fourier transform. Since $f(t)$ is real and zero for negative t, Equation (3) can be written as

$$f(t) = \frac{1}{\pi} \int_0^\infty F(j\omega)\, e^{j\omega T}\, d\omega \; f(t) = \text{real} \quad (3)$$

$$f(t) = \frac{2}{\pi} \int_0^\infty R(\omega) \cos \omega t\, d\omega \quad (18)$$

and

$$f(t) = -\frac{2}{\pi} \int_0^\infty I(\omega) \sin \omega t\, d\omega \quad (19)$$

These integrals, which express the inverse Fourier transform, are exactly the same as the integrals that express the direct transform, as given in Equation (11), except that t and ω are interchanged. $R(\omega)$ and $I(\omega)$ can thus be approximated by polynomial segments, and Equations (16) and (17) can be used to compute the integrals for the inverse transformation in the following manner:

$$R(\omega) \sim \sum_{i=1}^{n} u(\omega - W_i)\, [A_i' + B_i'(\omega - W_i) + C_i'(\omega - W_i)^2 + D_i'(\omega - W_i)^3 + \ldots] \quad (20)$$

where A_i', B_i', etc., refer to $R(\omega)$ and its derivatives. Therefore

$$f(t) \sim \frac{2}{\pi} \sum_{i=1}^{n} \left[-\frac{A_i'}{t} + \frac{2C_i'}{t^3} - \ldots \right] \sin tW_i + \left[-\frac{B_i'}{t^2} + \frac{6D_i}{t^4} - \ldots \right] \cos tW_i \quad (21)$$

In like manner $I(\omega)$ can be written

$$I(\omega) \sim \sum_{i=1}^{n} u(\omega - W_i)\, [A_i' + B_i'(\omega - W_i) + C_i'(\omega - W_i)^2 + D_i'(\omega - W_i)^3 + \ldots] \quad (22)$$

and $f(t)$ is given by

$$f(t) \sim -\frac{2}{\pi} \sum_{i=1}^{n} \left[-\frac{A_i'}{t} + \frac{2C'_i}{t^3} - \ldots \right] \cos tW_i - \left[-\frac{B_i'}{t^2} + \frac{6D_i'}{t^4} - \ldots \right] \sin tW_i \quad (23)$$

The relative advantages of using either Equation (21) or (23) for the evaluation of $f(t)$ have been discussed by Clements and Adler (3). In general, it is better to use Equation (23) for functions that have no discontinuity at the origin, while Equation (21) is better suited for inversion of functions with such a discontinuity.

Truncation

In many cases the functions $f(t)$ and $F(j\omega)$ have values that asymptotically approach zero as t and ω become large. As a result, for numerical transformation, the integrals involving the functions must be truncated at some point where the integrand is nonzero, and the remainder of the integral, from this point to infinity, is discarded. It is then pertinent to discuss the nature of the errors that occur when such truncated functions are numerically transformed or inverted.

Consider a time function $f(t)$ which has a Fourier transform $F(j\omega)$ over the entire frequency spectrum from zero to positive infinity. The numerical computation of the inverse Fourier transform, however, necessitates that the frequency spectrum be truncated at a finite point ω_c. The resulting expression $\overline{F}(j\omega)$ is then an approximation to $F(j\omega)$. It is exactly equal to $F(j\omega)$ over the interval 0 to ω_c but equal to zero for $\omega > \omega_c$. The inversion of $\overline{F}(j\omega)$ leads to an approximation $\overline{f}(t)$ of the original $f(t)$. It can easily be shown from Parseval's theorem that $\overline{f}(t)$ is the best estimate in the least squares sense, of $f(t)$ that can be made with the truncated frequency spectrum. The closeness with which $\overline{f}(t)$ matches $f(t)$ depends on the severity of frequency domain truncation. The process of truncation of $f(t)$ and of subsequent transformation into the frequency domain has an analogous property. Further information on these properties and on the general quantitative description of the truncation process may be found in reference 5.

AN EXAMPLE OF FREQUENCY DOMAIN MODEL EVALUATION

As a simple example of the procedure for evaluation of model parameters in the frequency domain, consider the following differential equation:

$$T\frac{dy}{dt} + y = x(t) \quad (24)$$

This equation describes the response of a linear first-order system excited by some arbitrary input $x(t)$. The Laplace transform solution is

$$Y_p(s) = X(s) \left(\frac{1}{Ts + 1} \right) \quad (25)$$

Substitution of $j\omega$ for s gives the Fourier transform solution.

$$Y_p(j\omega) = X(j\omega) \left(\frac{1}{j\omega T + 1} \right) \quad (26)$$

Substitution of Equation (26) into Equation (1) produces the frequency domain expression for ϕ for this particular problem.

$$\phi = \frac{1}{\pi} \int_0^\infty \left| Y_o(j\omega) - X(j\omega) \left(\frac{1}{j\omega T + 1} \right) \right|^2 d\omega \quad (27)$$

An approximation by the trapezoidal rule, which is usually satisfactory, yields

$$\phi \sim \frac{1}{2\pi} \sum_{k=2}^{M} [z_k(\omega_k) + z_{k-1}(\omega_{k-1})]\, [\omega_k - \omega_{k-1}] \quad (28)$$

where

$$z_k(\omega) = \left| Y_o(j\omega_k) - X(j\omega_k) \left(\frac{1}{j\omega_k T + 1} \right) \right|^2 \quad (29)$$

Figure 1 shows the experimental response observed when an analog computer simulation of a first-order system was excited by a triangular input pulse of 1-sec. duration and unit height. It is desired to make a least squares comparison of the observed response and the response predicted by a first-order transfer function. For the purpose of illustration, this response can be approximated by three linear segments. Table 1 shows how the coefficients in Equations (16) and (17) are calculated from the linear approximation. From the coefficients in this table the Fourier transform of the observed response may be written from Equations (16) and (17) as

$$Y_o(j\omega) = -\frac{1}{\omega^2}(0.425 - 0.645 \cos 0.8\omega + 0.165 \cos 1.8\omega + 0.0546 \cos 4.0\omega) + \frac{j}{\omega^2}(-0.645 \sin 0.8\omega + 0.165 \sin 1.8\omega + 0.0546 \sin 4.0\omega) \quad (30)$$

The Fourier transform of the input triangular pulse can be written similarly:

$$X(j\omega) = -\frac{1}{\omega^2}(2 - 4\cos 0.5\omega + 2\cos\omega) + \frac{j}{\omega^2}(-4\sin 0.5\omega + 2\sin\omega) \quad (31)$$

These equations do not give the values of $Y_o(j\omega)$ and $X(j\omega)$ for $\omega = 0$. These values must be calculated from the area under the respective $y_o(t)$ and $x(t)$ curves.

The values of ω_k to be used in Equation (29) are selected so that the variation of the right-hand side of the equation can be adequately represented over the frequency range of interest. An accurate solution for this example would require around 20 or 30 points from $\omega = 0$ to $\omega = \omega_{\max}$, where

$$\frac{|Y_o(j\omega)|_{\omega=\omega_{\max}}}{|Y_o(j\omega)|_{\omega=0}} \simeq 0.02 \quad (32)$$

A nonlinear, least squares algorithm, such as Marquardt's, can be used to minimize ϕ as given by Equation (28), and to find the best value of the system time constant T. It is important to notice that in the iterative minimization of ϕ, only $1/(j\omega_k T + 1)$ must be recalculated for each adjustment of T. The transforms of the input pulse and the observed response are not dependent on the parameter T and are only evaluated once.

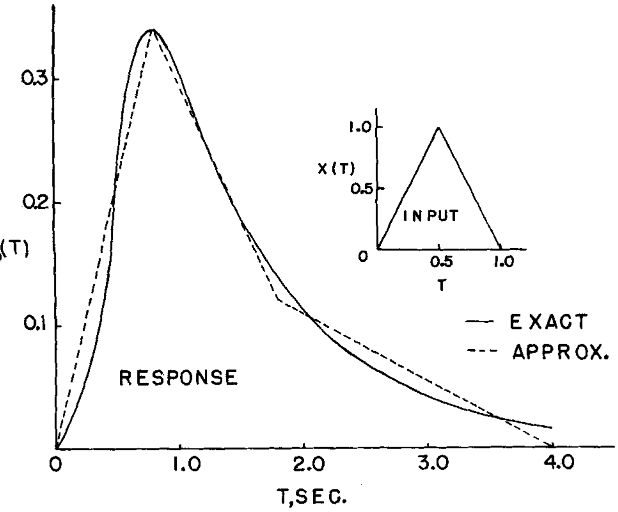

Fig. 1. Stimulus and response curves for a first-order system.

TABLE 1. CALCULATION OF RESPONSE DISCONTINUITIES

Break point	Observed response	Segment	Slope	Slope change	Index
T_i	$y_0(t)$			i	B_i
0	0			0.425	1
		1	0.425		
0.8 sec.	0.34			−0.645	2
		2	−0.22		
1.8 sec.	0.12			0.165	3
		3	−0.0546		
4.0 sec.	0			0.0546	4

Responses

It is helpful at this point to reflect on the restriction on responses useful in frequency domain modeling. The usual restriction for the existence of a Fourier transform applies to numerical transformation. However, certain important functions that are not directly transformable can be handled by an artifice. Consider an observed system response that has come to some steady state value at time zero and, after a disturbance, assumes a second steady state value. Strictly speaking, such a function is not Fourier transformable. However, if the y axis is shifted so that the initial steady state value is zero, the final steady state value can be labeled k_o, and the response written as

$$y_o(t) = k_o - [k_o - y_o(t)] \quad (33)$$

or

$$y_o(t) = k_o - f_o(t) \quad (34)$$

where

$$f_o(t) = k_o - y_o(t) \quad (35)$$

The predicted response can be written in the same manner to give

$$y_p(t) = k_p - f_p(t) \quad (36)$$

where

$$f_p(t) = k_p - y_p(t) \quad (37)$$

Now if ϕ is to be a meaningful measure of the deviation, the predicted results must have the same steady state gain as the observed results, that is, $k_p = k_o$. Thus, the time domain expression for ϕ becomes

$$\phi = \int_0^\infty [f_o(t) - f_p(t)]^2\, dt \quad (38)$$

The functions $f_p(t)$ and $f_o(t)$ are Fourier transformable, so the frequency expression for ϕ becomes simply

$$\phi = \frac{1}{\pi}\int_0^\infty |F_o(j\omega) - F_p(j\omega)|^2\, dt \quad (39)$$

The most common application for this approach is in modeling a system that has been excited by a step input.

ADVANTAGES OF FREQUENCY DOMAIN MODEL FITTING

1. The most important difficulty in the direct application of the nonlinear least squares technique to time domain expressions for the observed and predicted responses lies in the calculation of the predicted response $y_p(t)$. For rather simple systems with simple inputs, the calculation of $y_p(t)$ may offer no difficulty. For example, the response of the first-order system described by Equation (24) to a unit step input is easily found to be

$$y_p(t) = 1 - e^{-t/T} \quad (40)$$

However, for an arbitrary measured input $x(t)$, the response can only be written as a convolution of the arbitrary signal with the unit impulse response.

$$y_p(t) = x(t) * \frac{e^{-t/T}}{T} \quad (41)$$

or

$$y_p(t) = \int_0^t \frac{e^{-(t-\tau)/T}}{T} x(\tau)\, d\tau \quad (42)$$

If this method for the calculation of $y_p(t)$ is used in conjunction with the time domain minimization of ϕ, it will be necessary to perform numerically the integration in Equation (42) for each time point for each iterated value of the parameter T. For a more complicated model with a large number of parameters this can be quite a time consuming process, particularly when compared to the calculation of $y_p(j\omega)$ in the frequency domain.

The convolution indicated by Equations (41) and (42) becomes multiplication when these expressions are transformed to the frequency domain.

$$Y_p(j\omega) = X(j\omega)\left(\frac{1}{j\omega T + 1}\right) \quad (43)$$

Thus, for arbitrary inputs, the ease with which $Y_p(j\omega)$ can be evaluated makes the frequency domain minimization of ϕ much faster and simpler.

2. Another important advantage in frequency domain modeling is the facility with which analytical frequency solutions can be obtained as compared with time solutions. However, the analytical inversion of the frequency solution to find the time solution is formidable. Also, it is quite likely that such a solution would contain definite integrals of untabulated functions that would present special numerical evaluation problems.

3. For lumped parameter models there is no change in the form of the frequency solution as the values of the parameters change. However, the form of the time domain solution changes as the roots of the characteristic equation change from real to multiple to complex. Difficulties arise in the evaluation of the time solutions and their derivatives near the transition points.

4. The region of interest over which it is desired to fit a mathematical model is quite often conveniently expressed in the frequency domain. Frequency domain model evaluation allows one to take this into consideration by modifying the limits of the integral of the squared error to include only the region of interest. This may involve the elimination of a high- or low-frequency range or the rejection of a band of frequencies that perhaps contains noise or a spurious frequency component. In certain cases it may be desirable to weight the deviations as a function of frequency.

CONCLUSIONS

Mathematical modeling is often thought of as being concerned with time domain signals. However, for many problems it is much simpler and computationally advantageous to evaluate the model in the frequency domain. Indeed, for some problems it may be the only feasible approach. Another distinct advantage of frequency domain regression is that frequency domain specifications and restrictions can be easily incorporated.

The numerical Fourier transformation equations involved in frequency domain modeling are ideally suited for machine computation. This makes it possible to construct generalized computer programs useful in a broad class of problems, thus reducing the time and effort expended on specialized programs for individual modeling problems.*

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NOTATION

A_i, B_i, C_i, D_i = coefficients used to characterize $f(t)$
A_i', B_i', C_i', D_i' = coefficients used to characterize $F(j\omega)$
$f(t)$ = time domain function
$\bar{f}(t)$ = inverse of $\bar{F}(j\omega)$
$F(j\omega)$ = Fourier transform of $f(t)$
$\bar{F}(j\omega)$ = truncated Fourier transform of $f(t)$
$G_o(j\omega)$ = observed transfer function
$G_p(j\omega)$ = predicted transfer function
I_o = imaginary part of Fourier transform of Y_o
I_p = imaginary part of Fourier transform of Y_p
k_o = steady state response to a step change
R_o = real part of the Fourier transform of Y_o
R_p = real part of the Fourier transform of Y_p
s = Laplace transform variable
T = first-order time constant
T_i = time point in $f(t)$
t = time
W_i = frequency point in $F(j\omega)$
x = input variable
$X(j\omega)$ = Fourier transform of input function
y = output variable
Y_o = observed time domain output
Y_p = predicted time domain output

Greek Letters

ϕ = integral of the squared deviations
ω = frequency

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* Exemplary programs will soon be available in an Instrument Society of America publication.

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