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CHARACTERIZATION OF CALORIMETERS BY DIRECT CALCULATION OF THE RECURSION EQUATION COEFFICIENTS

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ABSTRACT

A new procedure for characterizing calorimeters is described in which the coefficients of the recursive equation modelling the calorimeter are calculated directly. The new method is considerably faster than previous least-squares techniques, even when more experimental thermogram points are used, and although it is more affected by noise, the coefficients it yields are valid for frequencies below those that are so affected.

INTRODUCTION

The deconvolution of the signals produced from properly characterized calorimeters is relatively straightforward, but the rapid, accurate characterization of calorimeters in the first place is still the subject of research. Whatever the deconvolution method employed, in subsequent work in which the calorimeter is used, the accuracy of the parameters characterizing it determine the quality of the deconvolution process, especially in time-varying systems, in which characterization errors are accumulative [1]. In recent years, several methods have been developed for determining the time constants of calorimeter systems, including the least-squares estimation of the unit pulse response [2,3] and the use of Padé approximations [4], modulating functions [5], Mellin deconvolution [6] or the z-transform [7]. In this article we present a new least-squares characterization method which, on a microcomputer, takes just a few minutes to approximate the coefficients of the calorimeter equation (as against the several hours taken by previous methods). The coefficients obtained can either be used directly for deconvolution by means of the discrete transfer function [2] or converted to time constants for use in other deconvolution procedures.

THEORETICAL BACKGROUND

As is well known, a calorimeter can be represented in the frequency domain by a transfer function of the form

$$H(s)=\prod_{i=1}^{m}(\tau_i^* s+1)\Big/\prod_{i=1}^{n}(\tau_i s+1) \qquad (m<n-2) \tag{1}$$

(as the sensitivity of calorimeters is easily calculated, this factor has been omitted here for simplicity, i.e. we assume its value to be unity). The equivalent of eqn. (1) in the time domain is the unit pulse response

$$h(t)=\sum_{i=1}^{n} A_i \exp(-t/\tau_i) \tag{2}$$

where

$$A_i=\tau_i^{n-m-2}\frac{\prod_{j=1}^{m}(\tau_i-\tau_j^*)}{\prod_{\substack{k=1\\k\neq i}}^{n}(\tau_i-\tau_k)} \tag{3}$$

(eqn. (2), like all other functions of time in this article, refers to $t \geqslant 0$; all such functions are defined as identically zero for $t<0$). Equation (2) shows that the coefficients τ_i can be regarded as the time constants characterizing the exponential processes within the calorimeter. Note that eqn. (2) does indeed correspond to a calorimeter with unit sensitivity ($H(0)=1$), as

$$\int_{-\infty}^{+\infty} h(t)\,\mathrm{d}t=\int_{-\infty}^{+\infty}\sum_{i=1}^{n} A_i \exp(-t/\tau_i)\,\mathrm{d}t=\sum_{i=1}^{n} A_i\tau_i=1 \tag{4}$$

Because in modern calorimetry thermograms are obtained by periodic computer-controlled sampling of the calorimeter output signal (see Fig. 1), our task is to find a discrete transfer function $H(z)$ that transforms a known discrete input $x[k]$ obtained by sampling the calorimeter input signal $x(t)$ with period T (so that $x[k]=x(kT)$) into a discrete signal $y[k]$ such that $y[k]=y(kT)$, where $y(t)$ is the calorimeter output signal. In other words,

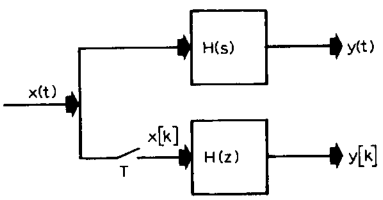

Fig. 1. Simulation of a system defined by $H(s)$ by means of a discrete system defined by $H(z)$. $x[k]=x(kT)$ and $y[k]=y(kT)$, where T is the sampling period.

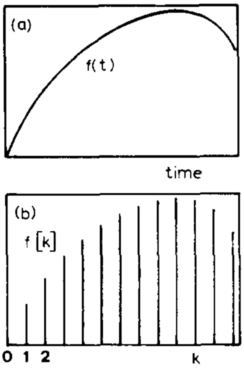

Fig. 2. An analog signal $f(t)$ (a) compared with the sequence of sampled values $f[k]$ (b). Clearly, the integral of $f(t)$ is in general different from the sum of the $f[k]$.

we wish to find the discrete transfer function $H(z)$ that characterizes a discrete system simulating the analogue system characterized by $H(s)$.

If $H(s)$ is known, the solution to the above problem is as follows [8]. Let $h[k]$ be the result of sampling the unit pulse response $h(t)$ with period T

$$h[k] = h(kT) = \sum_{i=1}^{n} A_i \exp(-kT/\tau_i) = \sum_{i=1}^{n} A_i (w_i)^k \tag{5}$$

where $w_i = \exp(-T/\tau_i)$. The sensitivity of the system defined by $h[k]$ is

$$M = \sum_{k=0}^{\infty} h[k] = \sum_{i=1}^{n} A_i \sum_{k=0}^{\infty} w^k = \sum_{i=1}^{n} A_i/(1 - w_i) \tag{6}$$

which in general is not unity (see Fig. 2). Approximating $w_i = \exp(-T/\tau_i)$ by $1 - T/\tau_i$ in fact yields $M = 1/T$, and we adopt as our discrete simulator the system defined by the unit pulse response

$$h[k] = M^{-1} \sum_{i=1}^{n} A_i \exp(-kT/\tau_i) = M^{-1} \sum_{i=1}^{n} A_i (w_i)^k \tag{7}$$

The desired discrete transfer function $H(z)$ is the z transform of $h[k]$

$$H(z) = \sum_{k=0}^{\infty} h[k] z^{-k} = M^{-1} \sum_{i=1}^{n} A_i z/(z - W_i) \tag{8}$$

$$= \frac{\sum_{i=0}^{n-1} b_i z^{n-1}}{\sum_{i=0}^{n} a_i z^{n-1}} = \frac{\sum_{i=0}^{n-1} b_i z^{-i}}{\sum_{i=0}^{n} a_i z^{-1}} \tag{9}$$

where $a_0 = 1$ and the other a_i and b_i terms are functions of the A_i, w_i and M terms.

If $X(z)$ and $Y(z)$ are the z transforms of $x[k]$ and $y[k]$ respectively, then $Y(z)=H(z)X(z)$, so that by eqn. (9)

$$X(z)\sum_{i=0}^{n-1} b_i z^{-i} = Y(z)\sum_{i=0}^{n} a_i z^{-i} \tag{10}$$

which is equivalent to the recursive time domain equation

$$y[k] + \sum_{i=1}^{n} a_i y[k-i] = \sum_{i=0}^{n-1} b_i x[k-i] \tag{11}$$

This equation allows the output sequence $y[k]$ to be constructed from the initial conditions and the input sequence $x[k]$; our task is to estimate the coefficients a_i and b_i, from which the time constants τ_i and τ_i^* can be obtained, if desired, via eqns. (9), (8) and (3) and the definition of the w_i.

ESTIMATION OF THE COEFFICIENTS

For large enough values of N, the a_i and b_i of eqn. (11) can be estimated as follows from known values of $y[k]$ and $x[k]$ for $k=0, \ldots, N$. The corresponding set of $N+1$ equations of the form of eqn. (11) (one for each value of k) can be written in matrix form as

$$FP = S \tag{12}$$

where

$$F = \begin{bmatrix} x[0] & x[-1] & \ldots & x[1-n] & -y[-1] & -y[-2] & \ldots & -y[-n] \\ x[1] & x[0] & \ldots & x[2-n] & -y[0] & -y[-1] & \ldots & -y[1-n] \\ & & & \cdots & \cdots & & & \\ x[N] & x[N-1] & \ldots & x[N-n+1] & -y[N-1] & -y[N-2] & \ldots & -y[N-n] \end{bmatrix} \tag{13}$$

$$P = (b_0\ b_1\ \ldots\ b_{n-1}\ a_1\ a_2\ \ldots\ a_n)' \tag{14}$$

$$\text{and } S = (y[0]\ y[1]\ \ldots\ y[N])' \tag{15}$$

(primes indicate the transpose operation); the least-squares estimation of the a_i and b_i amounts to finding the a_i and b_i that minimize the functional

$$I = \tfrac{1}{2}(S-FP)'(S-FP) \tag{16}$$

The desired values are given by

$$\frac{\delta I}{\delta P} = -F'S + F'FP = 0 \tag{17}$$

i.e.

$$P = (F'F)^{-1}F'S \tag{18}$$

The greater part of the time taken to compute P from eqn. (18) consists of the time taken to find the 'pseudo-inverse' matrix [8,9] $(F'F)^{-1}$, which is much shorter than the time required by methods that employ iterative non-linear estimation or the numerical calculation of Laplace transforms or z transforms.

TRIAL RESULTS

The characterization method described above was tested by computer simulation of a system of unit sensitivity defined by the parameters

$$\tau_1 = 200 \text{ s}, \quad \tau_2 = 90 \text{ s}, \quad \tau_3 = 10 \text{ s}, \quad \tau_1^* = 20 \text{ s}$$

The values of these parameters were estimated by the proposed method after simulating the output corresponding to each of three input signals: the delta function, the Heaviside function, and a pulse lasting 60 sampling periods. In each case, the first 300 samples of input and output were used for parameter estimation. The influence of sampling period on the accuracy of the method was investigated by performing the characterization for 1 s, 2.5 s and 5 s sampling periods. Figures 3a and 3b show the simulated input and output signals respectively.

As Table 1 shows, the best results were achieved by the longest sampling period. This is logical, as 300 five-second sampling periods cover 1500 s of signal, as against only 300 s of signal for the one-second sampling period; the longer sampling period therefore affords information concerning a greater length of signal. Sampling 1500 s of signal with a period of 1 s would of course enable much greater accuracy to be attained than by sampling every five seconds, but would be computationally much costlier. As it is, the results show that highly satisfactory accuracy is achieved with relatively few sample points so long as about $7\tau_1$ seconds of the input and output signals are covered. Table 1 also shows that though the best estimations were obtained using the delta function as input, very good estimates were also

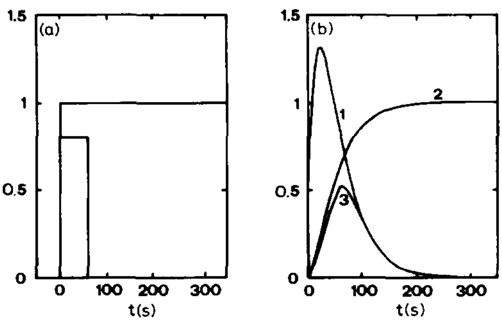

Fig. 3. Simulated input signals (a) used to test the proposed characterization method, and the corresponding simulated responses (b). (1) corresponds to the delta function input, (2) to the Heaviside (step) function and (3) to a $60T$ pulse.

TABLE 1

Results of using the proposed method, with various different input signals and sampling periods, to characterize a system whose true time constants were $\tau_1 = 200$ s, $\tau_2 = 90$ s, $\tau_3 = 10$ s and $\tau_1^* = 20$ s

T	delta	step	pulse	T	delta	step	pulse
	τ_1				τ_2		
1	195.834	236.266	212.710	1	90.959	83.508	87.171
2.5	200.917	203.501	201.526	2.5	89.800	89.258	89.665
5	199.991	199.629	199.623	5	90.002	90.080	90.085
	τ_3				τ_1^*		
1	9.999	9.966	9.981	1	20.003	19.876	19.925
2.5	10.000	9.999	9.998	2.5	20.018	19.997	19.995
5	10.000	10.000	10.002	5	20.073	20.000	20.003

afforded by the step function and pulse. This is a very pleasing result, because when it comes to feeding inputs into a real calorimeter, the delta function is much more difficult to provide than the other two, which are the signals commonly used in practice.

INFLUENCE OF NOISE

The influence of noise on the accuracy of the proposed method was studied by using it to characterize the same system as above using a Heaviside input signal and a 5 s sampling period when white noise was added to the output. Signal-to-noise ratios of 60, 70, 80, 90 and 100 dB were used in different runs.

The results (Table 2) show that the method is quite sensitive to noise. This was to be expected, as noise was not taken into account in the model used in developing it. The possibility of modifying it to take noise into account is currently being investigated. It may be pointed out, however, that in spite of the inaccuracy of the time constants for S/N ratios of less than 100 dB, the

TABLE 2

Results of using the proposed method, with a Heaviside input signal and a sampling period $T = 5$ s, to characterize the same system as in Table 1 with various levels of noise in the output

	S/N ratio (dB)				
	60	70	80	90	100
τ_1	225.641	216.677	210.772	205.591	200.592
τ_2	66.783	72.308	77.341	83.624	89.131
τ_3	–	–	4.271	6.962	9.661
τ_1^*	7.778	6.956	9.958	15.300	19.400

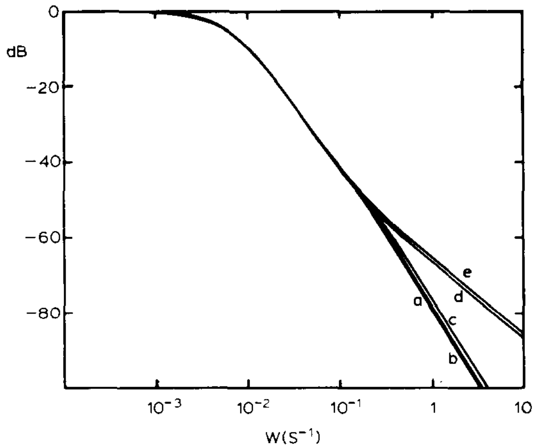

Fig. 4. Amplitudes of transfer functions obtained using noisy output signals. (a) $S/N = 100$ dB; (b) $S/N = 90$ dB (effectively identical to (a)); (c) $S/N = 80$ dB; (d) $S/N = 70$ dB; (e) $S/N = 60$ dB.

transfer function is only badly inaccurate at frequencies greater than those that in practice have a significant effect (Fig. 4), at least so long as $S/N > 80$ dB. For $S/N < 80$ dB, the lack of any meaningful estimate of τ_3 gives rise to additional constriction of the useful bandwidth.

CONCLUSIONS

The calorimeter characterization procedure described in this article affords the coefficients of the recursive equation equivalent to the calorimeter by a direct (non-iterative) calculation whose lengthiest stage is the inversion of a $2n \times 2n$ matrix (n being the number of poles of the system). Deconvolution of the output signals corresponding to unknown inputs is then immediate by means of the z transform. The procedure described is much faster than those developed hitherto, and is highly satisfactory when applied to signals with signal-to-noise ratios greater than 70 dB.

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