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DECONVOLUTION IN CONDUCTION CALORIMETERS: AN ANALYTICAL TREATMENT AND EXPERIMENTAL RESULTS FROM THE PULSED TRANSFER FUNCTION

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ABSTRACT

Various techniques may be employed to approximate thermogenesis in conduction calorimeters by studying the transfer function (harmonic analysis, time domain analysis, analogue and digital filters, etc.). This article describes the use of the pulsed transfer function and Truxal's method of compensation as a technique suitable for employing with data sampling systems in the low frequency domain. The theory developed is applied experimentally to a Calvet conduction calorimeter, which is shown to require a compensating plant.

INTRODUCTION

A continuous linear system may be characterized by a differential equation of the type [1]

$$\sum_{i=0}^{n} a_i \frac{d^i}{dt^i} y(t) = \sum_{j=0}^{m} b_j \frac{d^j}{dt^j} x(t) \tag{1}$$

where x(t) and y(t) are, respectively, the input and output of the linear system. The Laplace transform of a function f(t) is defined as

$$F(s) = \int_0^{\infty} f(t)\, e^{-st}\, dt \tag{2}$$

where s is complex. When the Laplace transform is applied to both sides of (1) we obtain

$$\sum_{i=0}^{n} a_i s^i Y(s) = \sum_{j=0}^{m} b_j s^j X(s) \tag{3}$$

where X(s) and Y(s) are the Laplace transforms of x(t) and y(t), respectively.

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The transfer function of the system is defined [2] by

$$H(s)=\frac{\sum_{j=0}^{m} b_j s^j}{\sum_{i=0}^{n} a_i s^i}=k\frac{\prod_{j=1}^{m}(s+c_j)}{\prod_{i=1}^{n}(s+p_i)} \tag{4}$$

where $-p_i$ $(i=1,2,\ldots,n)$ are the poles of the system, $-c_j$ $(j=1,2,\ldots,m)$ are the zeros, and $k=b_m/a_n$. In terms of the transfer function, eqn. (3) now adopts the form

$$Y(s)=H(s)\,X(s) \tag{5}$$

For the system to be stable the poles of $H(s)$ must lie in the half-plane $R_e(s)<0$, and in a physically real system the number of zeros must be less than or equal to the number of poles, i.e. $m<n$. We shall restrict the present summary to the case of real poles of multiplicity one. The extension to complex poles of higher multiplicity is immediate. In terms of the time constants τ_{0j} and τ_{1j} corresponding, respectively, to the zeros and the poles of $H(s)$, eqn. (4) becomes

$$H(s)=k\frac{\prod_{i=1}^{n}\tau_{1i}}{\prod_{j=1}^{m}\tau_{0j}}\,\frac{\prod_{j=1}^{m}(\tau_{0j}s+1)}{\prod_{i=1}^{n}(\tau_{1i}s+1)} \tag{6}$$

where

$$\tau_{0j}=\frac{1}{c_j}\qquad (j=1,2,\ldots,m)$$

$$\tau_{1i}=\frac{1}{p_i}\qquad (i=1,2,\ldots,n) \tag{7}$$

Deconvolution consists in finding the input $x(t)$ of the system given $y(t)$, the output. Since from eqn. (5)

$$X(s)=H^{-1}(s)\,Y(s) \tag{8}$$

the problem posed is to find an expression for $H^{-1}(s)$ that is both stable and physically possible.

THE PULSED TRANSFER FUNCTION

When a data sampling system is employed to record the output of the system under study, knowledge of $y(t)$ is limited to a sequence of values $y(kT)$ $(k=1,\ldots,N)$ where T is the interval between samples, and NT is the total period over which sampling takes place. Under these conditions the linear system being studied must be treated as discrete, and instead of by (1) is characterized by a difference equation of the form [3]

$$\sum_{i=0}^{n} a_i y(k-i) = \sum_{j=0}^{m} b_j x(k-j) \tag{9}$$

where for f = x, y $f(k-i)$ is short for $f[(k-i)T]$.

The discrete equivalent of (2) is

$$F(z) = \sum_{k=0}^{\infty} f(k)\, z^{-k} \tag{10}$$

which, applied to (9) produces

$$Y(z) = H(z)\, X(z) \tag{11}$$

$H(z)$ is the pulsed transfer function [3], the poles of which must lie within the unit circle in the z plane if the system is to be stable. The deconvolution problem is now to find a stable, physically possible $H^{-1}(z)$ such that

$$X(z) = H^{-1}(z)\, Y(z) \tag{12}$$

THE BILINEAR TRANSFORMATION

Equation (6) can be expressed in the form

$$H^{-1}(s) = \frac{1}{M} \frac{\prod_{i=1}^{n} (\tau_{1i} s + 1)}{\prod_{j=1}^{m} (\tau_{0j} s + 1)} \tag{13}$$

where

$$M = k \frac{\prod_{i=1}^{n} \tau_{1i}}{\prod_{j=1}^{m} \tau_{0j}} \tag{14}$$

is the steady-state gain of the system. $H^{-1}(z)$ can be obtained directly from $H^{-1}(s)$ by applying the bilinear transformation defined by [4]

$$s \rightarrow \frac{2}{T} \frac{1 - z^{-1}}{1 + z^{-1}} \tag{15}$$

which transforms the half-plane $R_e(s) < 0$ into the unit disc in the z plane, the imaginary axis into the unit circle and the half-plane $R_e(s) > 0$ into the region $|z| > 1$ of the z plane.

Since the poles of $H^{-1}(s)$ are the zeros of $H(s)$, for the former to be stable the zeros of the latter must lie in the half-plane $R_e(s) < 0$, whence the bilinear transformation maps then into the region $|z| < 1$. The pulsed transfer function $H^{-1}(z)$ has m poles and n zeros, with $m < n$, but if $m < n$, $H^{-1}(z)$

is not physically possible; it may be modelled on a computer but will present undesirable oscillations.

TRUXAL'S METHOD OF COMPENSATION

When $m < n$, $H^{-1}(z)$ may be multiplied by Truxal's compensation factor [1,2] so as to arrive at a function representing a physically possible system with the same steady-state gain as $H^{-1}(s)$ itself. This function, which must have $n-m$ poles, may be considered as representing a physical compensating plant. It is defined by

$$G(s) = k' \prod_{q=m+1}^{n} \tau_{0q} \frac{1}{\prod_{q=m+1}^{n} \left(\tau_{0q} s + 1\right)} \tag{16}$$

where

$$k' = \frac{1}{\prod_{q=m+1}^{n} \tau_{0q}} \tag{17}$$

to ensure that the steady-state gain is not altered. The $n-m$ poles added by $G(s)$ should be so much greater than those of $H^{-1}(s)$ (τ_{0q} so small) as not to have an appreciable effect upon the low-frequency behaviour of the system at the same time as they avoid uncontrolled oscillations.

As a result of the above we may write

$$\hat{X}(s) = \hat{G}(s)\, Y(s) \tag{18}$$

where $\hat{X}(s)$ is the low-frequency approximation to $X(s)$ and

$$\hat{G}(s) = H^{-1}(s)\, G(s) = \frac{1}{M} \frac{\prod_{i=1}^{n} \left(\tau_{1i} s + 1\right)}{\prod_{j=1}^{n} \left(\tau_{0j} s + 1\right)} \tag{19}$$

When transformed by (15) we obtain

$$\hat{G}(z) = \frac{1}{M} \frac{\prod_{i=0}^{n} \Gamma_{1i} z^{-i}}{\prod_{j=0}^{n} \Gamma_{0j} z^{-j}} \tag{20}$$

where the Γ_{ik} are coefficients whose full expression depends on the degree n of the polynomial. For $n = 3$, for example

$$\Gamma_{i0} = \prod_{j=1}^{3} \beta_{ij}$$

$$\Gamma_{i1} = \sum_{j=1}^{3} \alpha_{ij} \left(\prod_{\substack{k=1 \\ k \neq j}}^{3} \beta_{ik} \right)$$

$$\Gamma_{i2} = \sum_{j=1}^{3} \beta_{ij} \left(\prod_{\substack{k=1 \\ k \neq j}}^{3} \alpha_{ik} \right)$$

$$\Gamma_{i3} = \prod_{j=1}^{3} \alpha_{ij} \qquad (i = 0, 1) \tag{21}$$

where

$$\alpha_{ij} = T - 2\tau_{ij}$$

$$\beta_{ij} = T + 2\tau_{ij} \tag{22}$$

Equation (18) is now transformed to

$$\hat{\mathrm{X}}(z) = \hat{\mathrm{G}}(z)\, \mathrm{Y}(z) \tag{23}$$

i.e. by (20)

$$\hat{\mathrm{X}}(z) = \frac{1}{M} \frac{\sum_{i=0}^{n} \Gamma_{1i} z^{-i}}{\sum_{j=0}^{n} \Gamma_{0j} z^{-j}} \mathrm{Y}(z) \tag{24}$$

Finally, $\hat{x}(k)$ is obtained from $\hat{\mathrm{X}}(z)$ by carrying out the inverse-discrete Laplace transform.

$$z^{-j}\mathrm{F}(z) \rightarrow \mathrm{f}(k - j) \tag{25}$$

where the factor z^{-j} introduces a lag j in the function $\mathrm{f}(k)$.

DECONVOLUTION

After applying the inverse transform to both sides of (24) we find that

$$\hat{x}(k) = \frac{1}{\Gamma_{00}} \left[\frac{1}{M} \left(\sum_{i=0}^{n} \Gamma_{1i} y(k - i) \right) - \sum_{j=1}^{n} \Gamma_{0j} \hat{x}(k - j) \right] \tag{26}$$

This gives the low-frequency approximation at time kT in terms of the output for that and the preceding n sample times together with the approximations calculated for the latter.

To test this method of deconvolution we have fed the input $x(t)$ of Fig. 1 into the linear system described by the transfer function

$$\mathrm{H}(s) = 10^{-5} \frac{s + 0.25}{(s + 0.0025)(s + 0.01)(s + 0.1)} \tag{27}$$

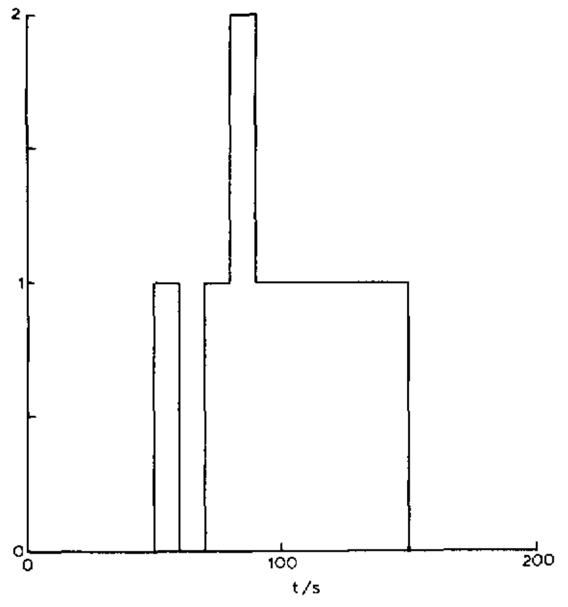

Fig. 1. Actual thermogenesis (the Y axis is in arbitrary units).

The computed output for a sampling interval of 1 s is shown in Fig. 2. In both Figs. the ordinates are in terms of the same arbitrary units. If this output is deconvoluted directly with $H^{-1}(z)$ without any compensating

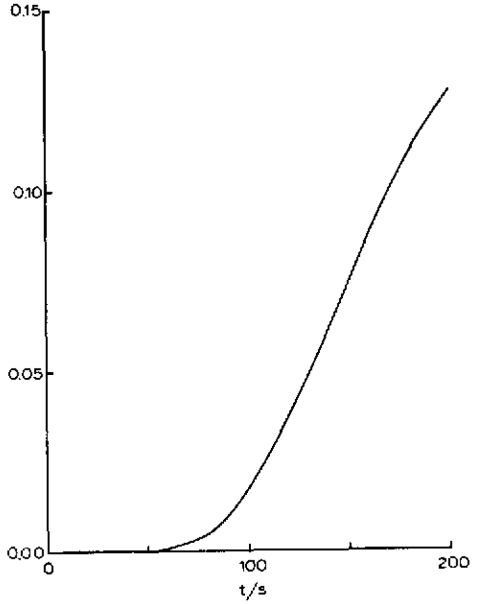

Fig. 2. Output of the system $H(s) = 10^{-5} s + 0.25/(s + 0.0025)(s + 0.01)(s + 0.1)$ for the input of Fig. 1 (the Y axis is in arbitrary units).

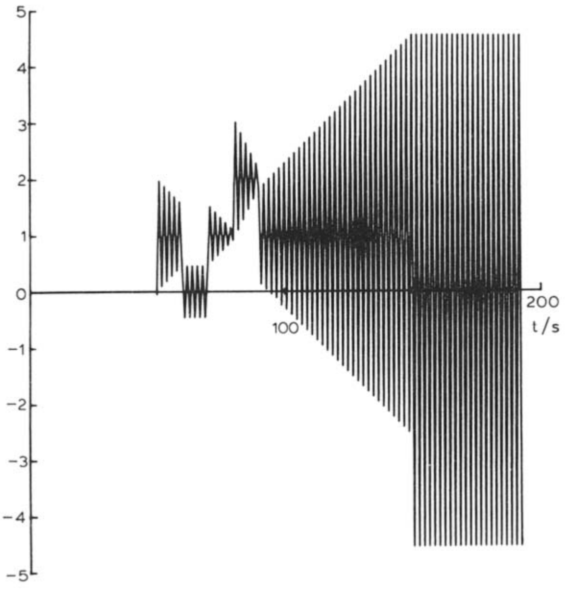

Fig. 3. Deconvolution by pulsed transfer function without Truxal's compensation (the *Y*-axis is in arbitrary units).

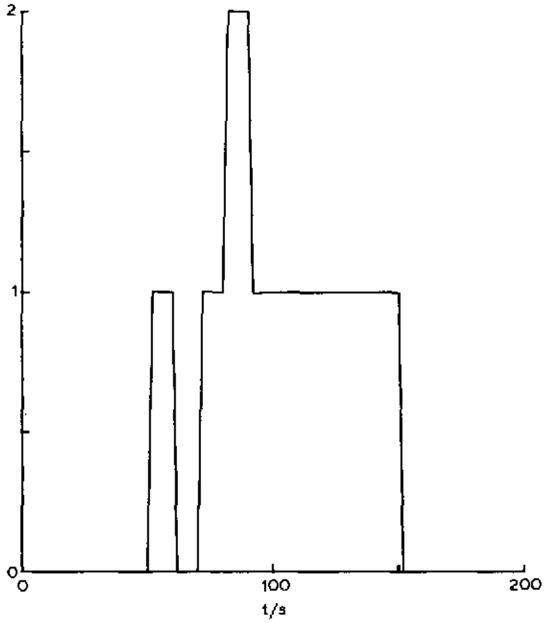

Fig. 4. Deconvolution by pulsed transfer function with Truxal's compensation. The compensating zeros are defined by $\tau_{02} = \tau_{03} = 1$ s.

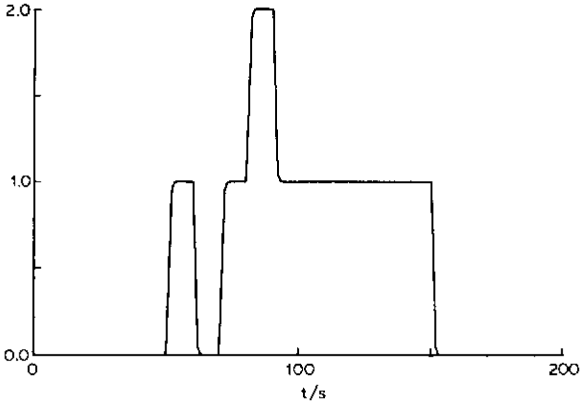

Fig. 5. Deconvolution by pulsed transfer function with Truxal's compensation. Overcompensation with $\tau_{02} = \tau_{03} = 1.5$ s is shown.

poles, the result is as shown in Fig. 3, which is stable but undergoes undesirable oscillations. However, if Truxal's method is applied, using the compensating time constants

$$\tau_{02} = \tau_{03} = 1\ s \tag{28}$$

the result obtained is that of Fig. 4. Figure 5 shows the result of overcompensation using the time constants $\tau_{02} = \tau_{03} = 1.5$ s and Fig. 6 undercompensation by the constants $\tau_{02} = \tau_{03} = 0.5$ s.

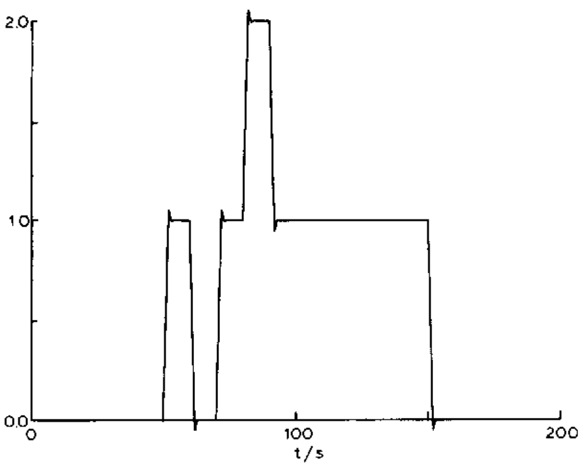

Fig. 6. Deconvolution by pulsed transfer function with Truxal's compensation. Undercompensation with $\tau_{02} = \tau_{03} = 0.5$ s is shown

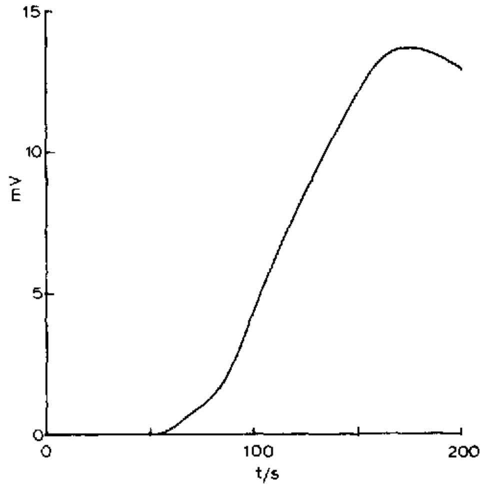

Fig. 7. The output thermogram corresponding to the input of Fig. 1 with Y axis unit = 0.8 W.

APPLICATION TO A PHYSICAL SYSTEM

The techniques described above were used to investigate the performance of a Calvet conduction microcalorimeter with stainless steel cells containing an axial resistance inside. An HP-3052-A data sampling system was used, which in combination with a stabilized power source can be programmed to generate any type of input to the calorimeter at the same time as it reads the output voltage once a second and stores it on magnetic tape.

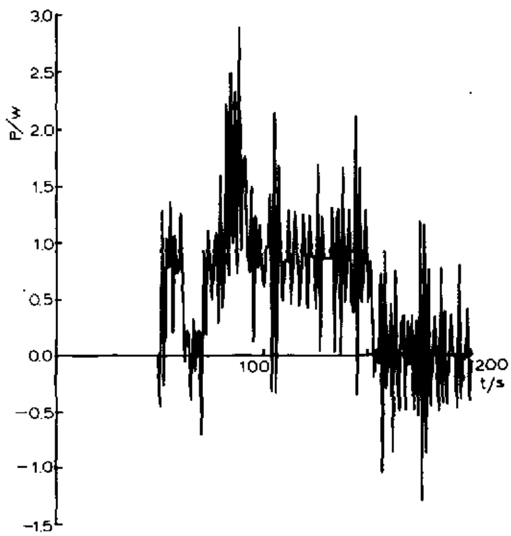

Fig. 8. Deconvolution of the thermogram of Fig. 7 without Truxal's compensation.

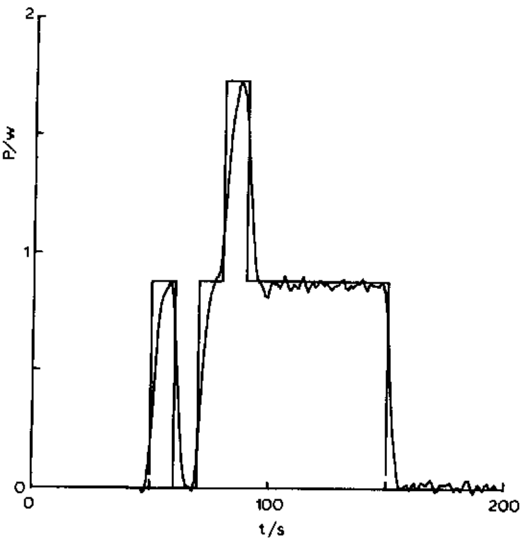

Fig. 9. Deconvolution of the thermogram of Fig. 7 with Truxal's compensation. Actual thermogenesis is also shown.

The calorimeter was modelled using a linear system with no zeros and three poles [5,6], with the following time constants

$$\tau_{11} = 237.0\ s$$
$$\tau_{12} = 12.3\ s \qquad (29)$$
$$\tau_{13} = 4.1\ s$$

and a steady-state gain of 48630×10^{-6} V W^{-1} with the input signals shown in Fig. 9, similar to that of Fig. 1 but with amplitudes of 0.8 and 1.7 W, the outputs were as shown in Fig. 7. If these outputs are deconvolved using $H^{-1}(z)$ without compensation the results are as in Fig. 8, which shows the expected undesirable oscillations. However, if a compensating plant with the time constants

$$\tau_{01} = \tau_{02} = \tau_{03} = 1.5\ s \qquad (30)$$

is used, (26) results in the approximation to the real thermogenesis shown in Fig. 9.

CONCLUSIONS

The use of the pulsed transfer function and Truxal's method of compensation allows deconvolution of low-frequency calorimeter signals with a high degree of precision. In the present study 10 s signals from a Calvet conduction microcalorimeter were deconvolved after sampling once a second. The deconvolution technique presented is considered to be particularly suitable for use with the data sampling systems employed ever-increasingly in calorimetry.

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