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THERMOGENESIS: COMPARATIVE EFFICIENCY OF DECONVOLUTION BASED ON OPTIMAL CONTROL AND INVERSE FILTERS

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ABSTRACT

A general deconvolutive method developed from Optimal Control Theory is presented and applied to flux or conduction calorimetry. It requires a previous identification of the system and gives very similar results to equivalent inverse filters (i.e. using the same model). Nevertheless, on the one hand the thermogenesis has to be obtained off-line (inverse filters allow on-line deconvolution) but on the other, the method can handle time-varying systems.

INTRODUCTION

The present paper proposes a new deconvolution method in conduction calorimetry which is based on a technique developed in Automatics: Optimal Control Theory concerning a tracking problem [1]. The basis of the method is described and the mathematical tools are established. An identification procedure of the transfer function of a calorimetric device is then explained [2] so as to test this deconvolutive technique in flux calorimetry. The results obtained are compared with those given by equivalent inverse filters.

DECONVOLUTION AND OPTIMAL CONTROL

Let $y(t)$ be the response given by a certain experimental system (signal which is recorded by the measuring apparatus) corresponding to an input

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signal $u(t)$. If the device behaves linearly, let $\mathrm{TF}(t)$ be its impulse response (transfer function). Then the following convolution equation

$$y(t) = u(t) * \mathrm{TF}(t)$$

holds. The equivalent block diagram is shown in Fig. 1.

Very many deconvolutive techniques build up or develop a new system, linear or not, in series with the experimental system in such a way that the resultant output signal is the best approximation to the actual input $u(t)$ (Fig. 2). This is the case, for instance, for inverse filters [3,4]. In most cases, however, we lack any precise information on $u(t)$ so we can adopt a somewhat different method: we look for a certain $\hat{u}(t)$ whose convolution with $\mathrm{TF}(t)$ produces a good approximation $\hat{y}(t)$ to the actual response $y(t)$. Figure 3 illustrates such a procedure.

In order to test the quality of the response $\hat{y}(t)$ calculated, a criterium in terms of the error function $\epsilon(t) = y - \hat{y}$ will be defined. Consequently, the deconvolutive technique presented in this paper is based on the following facts: a given input signal $\hat{u}(t)$ gives rise, through a model of the system, to a response $\hat{y}(t)$ which should be as close as possible to the actual output signal recorded $y(t)$. We accept now that $\hat{u}(t)$ will be a valid approximation to the actual input $u(t)$. In other words, we deal with a function $\hat{y}(t)$ which pursues a reference function $y(t)$. This is a well-known problem in the frame of Automatics [5].

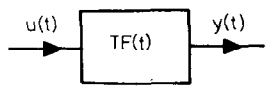

Fig. 1. Block diagram of the linear system defined by $\mathrm{TF}(t)$. $y(t)$ is the response to the input $u(t)$.

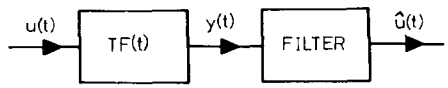

Fig. 2. Block diagram of the on-line inverse filter.

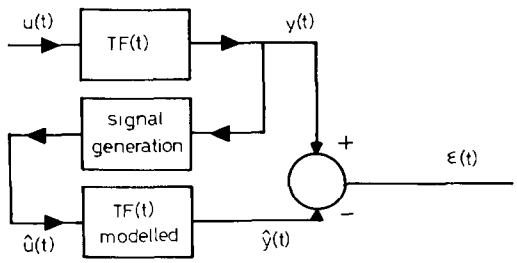

Fig. 3. Schematic representation of the tracking problem. $\hat{u}(t)$ is the simulated input which gives rise to the ouput $\hat{y}(t)$ through a model of the system. $\epsilon(t)$ is the error function to be minimized.

Firstly, we represent the system by means of its state equation rather than by its transfer function. Now, the state equation is a matrix expression equivalent to the differential equation which rules the process under study [5]. An example of how the state equation can be calculated from a model for the TF is shown in Appendix 1.

Generally speaking, whether the system changes in time or not, we may express its state equation as follows

$$\dot{\mathbf{x}} = A(t)\mathbf{x} + B(t)u$$

$$y = C(t)\mathbf{x}$$

where, $\mathbf{x} \in \mathbb{R}^n$, $u \in \mathbb{R}$, $y \in \mathbb{R}$, n being the order of the system; A, B, C are matrices of proper dimensions; $\mathbf{x}$ is the state vector associated with the A, B, C matrices; u is the input, and y is the output.

If we assume that our model is exact, then

$$\dot{\hat{\mathbf{x}}} = A(t)\hat{\mathbf{x}} + B(t)\hat{u}$$

$$\hat{y} = C(t)\hat{\mathbf{x}}$$

Now, we can state the problem as how to calculate $\hat{u}$ so that it would minimize a given efficiency criterium. The more convenient choice is

$$J = \tfrac{1}{2}\int_0^T \left[q(t)\epsilon^2 + r(t)\hat{u}^2\right] \mathrm{d}t$$

where $q(t) \geqslant 0$, $r(t) > 0$ $\forall t \in [0,T]$, because it leads by straightforward calculus of variations [5] to an analytical solution

$$\hat{u}^* = \frac{1}{r}{}^T B(\mathbf{v} - K\mathbf{x})$$

where $K(t)$ is a symmetric matrix verifying a Riccati equation

$$\dot{K} = -KA - {}^T AK + KB\frac{1}{r}{}^T BK + {}^T CqC$$

$$K(T) = 0$$

and $\mathbf{v}(t)$ is a vector defined by the linear equation

$$\dot{\mathbf{v}} = -{}^T\left(A - B\frac{1}{r}{}^T BK\right)\mathbf{v} - {}^T Cqy$$

$$\mathbf{v}(T) = 0$$

It should be noted that both differential equations must be solved by backward integration because the constraints refer to the time T where the process ends. This is why the second equation requires the whole output $y(t)$ and consequently an on-line deconvolution cannot be carried out. This deconvolutive procedure finally results in solving the afore-mentioned set of differential equations and its applicability includes systems changing in time.

IDENTIFICATION OF THE MODEL

The state equation of the calorimetric system may be obtained, concerning a time-independent system, from an analytical model of its transfer function. One simple way of obtaining such a model deals with the plot of the response to a step input.

Hudzovic's method [2]

The response to a step input is obtained by numeric integration (trapezoidal rule) of the experimental pulse response. Figure 4 shows both outputs: the impulse response and its corresponding integration. Hudzovic's method now yields a transfer function of any order where all the time constants are different. It starts by drawing the tangent to the inflexion point. This procedure allows calculation of the parameters δ, T_u, T_n and the delay τ. These parameters together with the characteristic abacus of the method give the order of the transfer function and the different time constants. In our case we obtain a third-order model whose transfer function

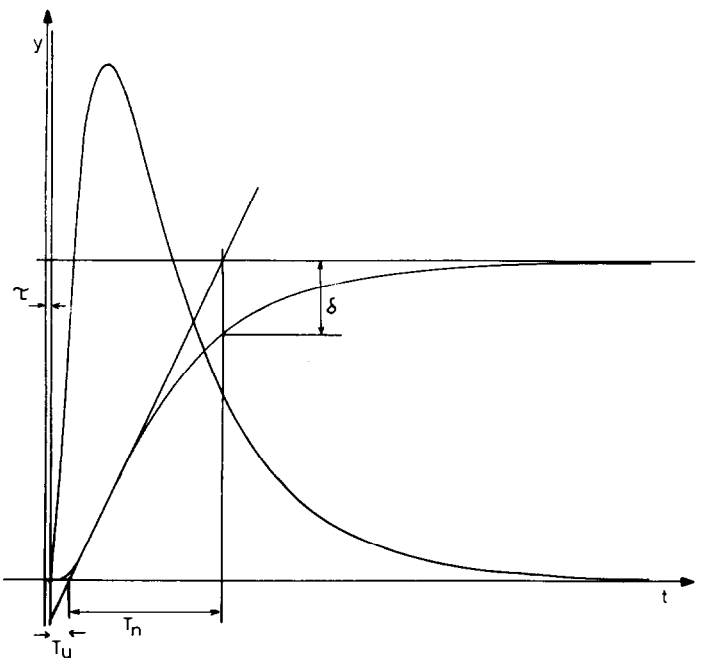

Fig. 4. Pulse and step response of the experimental system. The latter has been obtained by integrating the former. It is also schematically shown how to obtain the parameters δ, T_u, T_n, and τ used in the Hudzovic's identification method (see ref. 2).

reads

$$G(s) = \frac{e^{-12.5s}}{(1 + 189s)(1 + 43s)(1 + 25s)}$$

The exponential term in $G(s)$ accounts for a pure delay (or dead time) of 12.5 s in the experimental response.

APPLICATION TO CONDUCTION CALORIMETRY

This deconvolutive technique is now used to calculate the thermogenesis from various experimental records obtained from a flow or conduction calorimeter whose transfer function has been previously modelled. If the power is released far from the thermoelements, the transfer function consists only of poles [6], so Hudzovic's method is well suited to the identification of the system. The model of transfer function obtained has already been given. If the power is released near the detector system, the transfer function includes zeros which cannot be neglected. Hudzovic's method then fails to give the transfer function. Let us consider in this case

$$G(s) = \frac{(1 + 64s)(1 + 6s)}{(1 + 192s)(1 + 49s)(1 + 9s)}$$

This model has been obtained from the experimental transfer function corresponding to a power released near the detector system. The method has been discussed elsewhere [4,6]. Figure 5 compares modulus and phase in frequency space, $s = 2\pi j\nu_1$, of both analytical models and the corresponding transfer functions which are obtained by Fourier Transformation, through the FFT routine, of the experimental pulse responses.

As mentioned earlier, the first step after having chosen the model for the transfer function should be to write the state equation of the system. To this purpose we take the phase variables to be the state variables

$$x_1 = y \qquad x_2 = \dot{y} \qquad x_3 = \ddot{y}$$

Then the state equations are (see Appendix 1 for detailed calculations)

(1) Axial dissipation

$$\dot{\mathbf{x}} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -0.03937 & -0.50597 & -1.37094 \end{bmatrix} \mathbf{x} + \begin{bmatrix} 0 \\ 0 \\ 0.03937 \end{bmatrix} u$$

$$y = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \mathbf{x}$$

(2) Dissipation near the detector system

$$\dot{\mathbf{x}} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -0.0945 & -1.1810 & -2.7345 \end{bmatrix} \mathbf{x} + \begin{bmatrix} 0 \\ 0 \\ 0.0945 \end{bmatrix} u$$

$$y = \begin{bmatrix} 1 & 3.5 & 0.96 \end{bmatrix} \mathbf{x}$$

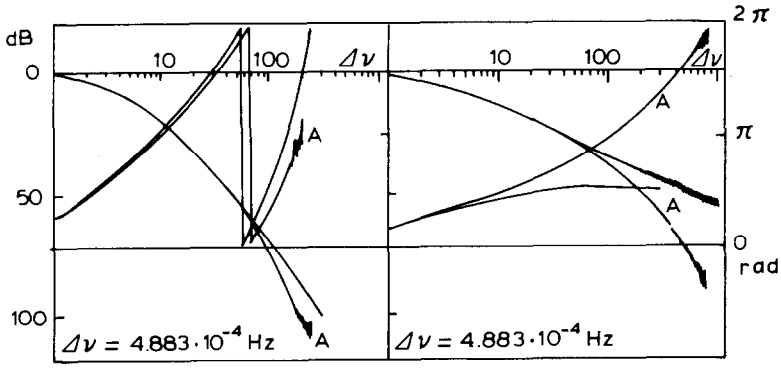

Fig. 5. Comparison between the experimental TF(s) (A) and the corresponding model $G(s)$. Left: Axial dissipation. Right: Dissipation near the detector system.

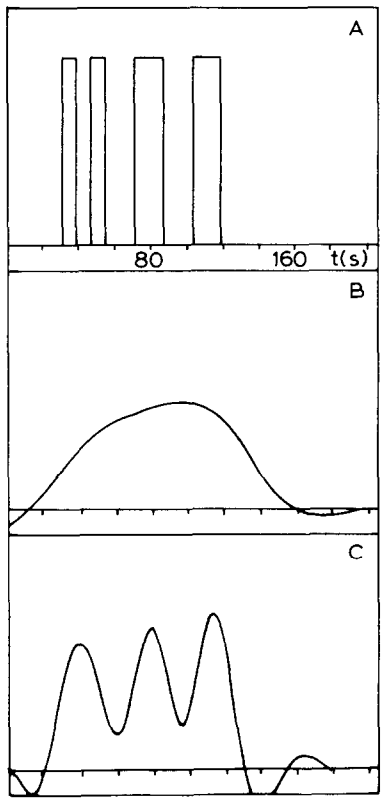

Fig. 6. How the choice of the parameter r influences the calculated thermogenesis. (A) Power released at an axial heating resistence in the calorimeter JLM-E1. We have used a sequence of four rectangular pulses of 15.76 mW whose widths are 8 s, 8 s, 16 s, and 16 s, respectively, separated by the same interval of time (measurement L96). (B) Reconstructed thermogenesis $\tilde{u}^*$ corresponding to $r = 2 \times 10^{-4}$. (C) Reconstructed thermogenesis $\tilde{u}^*$ corresponding to $r = 3 \times 10^{-6}$.

During the calculus the effective time scale has been contracted 20 times to avoid numeric problems in handling the matrices A, B and C. The matrices given above are already referred to the new scale. This choice of scale will also obviously affect the time constants of the model. The parameter q has been set equal to 1 and, in order to save memory occupation, $K(0)$ is calculated from $K(T)$ through backward integration, and then K is assumed to be constant [$K(t) = K(0)\ \forall t$] when calculating $\hat{u}^*$. This is quite a good approximation within the interval $(0, 4T/5)$, which is enough to obtain the thermogenesis. Figure 6 shows how critical the choice of r in the efficiency criterium can be.

The results given by this method have been compared with those corresponding to equivalent inverse filters, i.e. filters consisting of the same poles and zeros which define our present model [3,4]. Figure 7 shows the thermogenesis corresponding to different sequences and different locations of the heat sources. The results from the same thermograms, under equivalent conditions, are similar. A previous smoothing of the thermogram could

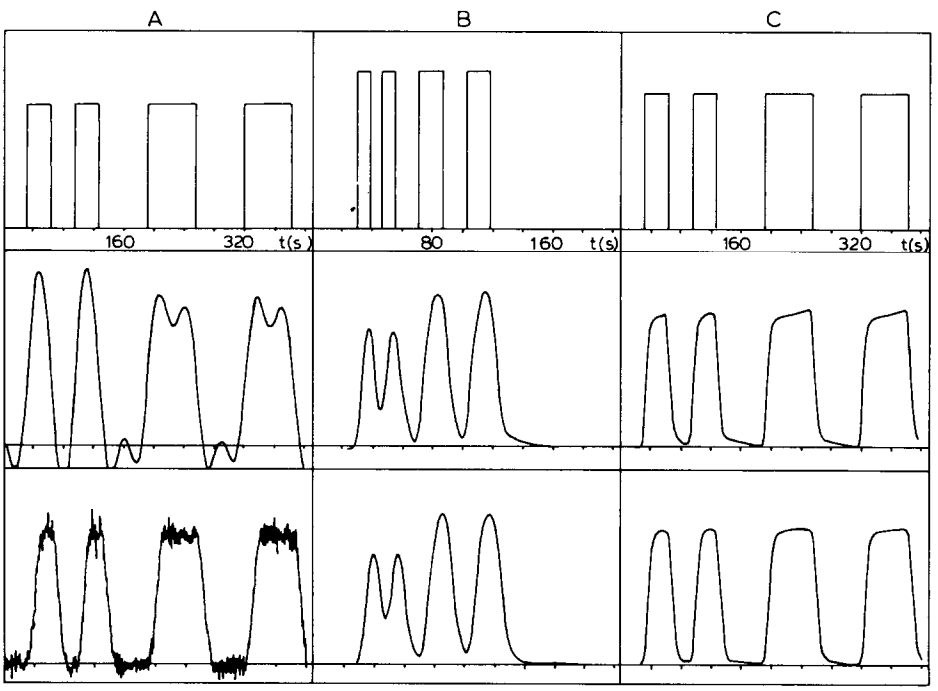

Fig. 7. Three different sequences of input pulses and the corresponding deconvolution: pursuit method (middle) and numeric inverse filtering (down). (A) Axial dissipation (measurement A3). Power released $W = 3.956$ mW. Sequence of 32 s–32 s–64 s–64 s; $r = 3 \times 10^{-6}$. (B) Dissipation near the detector system (measurement L99) Power released $W = 10.08$ mW. Sequence of 8 s–8 s–16 s–16 s; $r = 2 \times 10^{-4}$. (C) Dissipation near the detector system (measurement A4) Power released $W = 5.696$ mW. Sequence of 32 s–32 s–64 s–64 s; $r = 2 \times 10^{-4}$.

suppress the fluctuations which appear in the result.

The pursuit deconvolution method does not allow an on-line reproduction of the thermogenesis but it is equally sensitive to the experimental noise as inverse filters. However, the method is based on state equations, thus allowing for further generalization to non-stationary systems when the state matrices are time-dependent. Non-stationary systems are just beginning to be dealt with in flux calorimetry both theoretically and experimentally [7].

CONCLUSIONS

A general off-line deconvolutive method developed from Optimal Control Theory, which can be applied to a wide variety of deterministic linear systems, has been presented and tested on experimental records given by flux or conduction calorimeters. The method requires a previous model or identification of the system carried out, in our case, through standard graphic techniques. The efficiency criterion which has actually been chosen leads to an analytical solution of the problem, thus avoiding iterative calculus. The existence of experimental noise does not hamper the application of the method; on the other hand, it admits further generalization to deal with time-varying systems.

APPENDIX 1

How to calculate the state matrix

We start from a model for the transfer function of the system. We will restrict ourselves to a third-order system but generalization to higher order systems is straightforward.

Let us first consider a transfer function consisting only of three poles

$$G(s) = \frac{Y(s)}{U(s)} = \frac{1}{(1+\tau_1 s)(1+\tau_2 s)(1+\tau_3 s)}$$

The denominator may be rewritten to

$$G(s) = \frac{1}{\alpha s^3 + \beta s^2 + \gamma s + 1}$$

with

$$\alpha = \tau_1\tau_2\tau_3 = \prod_{i=1}^{3} \tau_i$$

$$\beta = \tau_1\tau_2 + \tau_1\tau_3 + \tau_3\tau_2 = \sum_{i<j} \tau_i\tau_j$$

$$\gamma = \tau_1 + \tau_2 + \tau_3 = \sum_{i=1}^{3} \tau_i$$

The transfer function is then

$$U(s) = \{\alpha s^3 + \beta s^2 + \gamma s + 1\}Y(s)$$

The inverse transform of this expression, if $y(t)$ and its first derivatives are zero at $t = 0$, yields

$$u(t) = \alpha \dddot{y} + \beta \ddot{y} + \gamma \dot{y} + y$$

Taking for granted the following state equation

$$\dot{\mathbf{x}} = A\mathbf{x} + Bu$$
$$y = C\mathbf{x}$$

and choosing as state variables

$$x_1 = y \qquad x_2 = \dot{y} \qquad x_3 = \ddot{y}$$

the matrices A, B and C are given by

$$\dot{\mathbf{x}} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1/\alpha & -\gamma/\alpha & -\beta/\alpha \end{bmatrix}\mathbf{x} + \begin{bmatrix} 0 \\ 0 \\ 1/\alpha \end{bmatrix} u$$

$$y = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}\mathbf{x}$$

Note that this equation is equivalent to the differential equation given above.

Secondly, if the model consists of poles and zeros

$$G(s) = \frac{Y(s)}{U(s)} = \frac{(1 + \tau^*{}_1 s)(1 + \tau^*{}_2 s)}{(1 + \tau_1 s)(1 + \tau_2 s)(1 + \tau_3 s)}$$

it can be decomposed into

$$G(s) = \frac{Y(s)}{U(s)} = \frac{Y(s)}{V(s)} \frac{V(s)}{U(s)}$$

with

$$\frac{V}{U} = \frac{1}{(1 + \tau_1 s)(1 + \tau_2 s)(1 + \tau_3 s)}$$

$$\frac{Y}{V} = (1 + \tau^*{}_1 s)(1 + \tau^*{}_2 s)$$

Let us choose now as state vector

$$x_1 = v \qquad x_2 = \dot{v} \qquad x_3 = \ddot{v}$$

The inverse Laplace transform of V/U leads to the same result as before, so the matrices A and B remain unchanged. But, concerning the zeros, let us write

$$Y = (1 + \tau_1^* s)(1 + \tau_2^* s)V = \{\phi s^2 + \psi s + 1\}V$$

from which $\phi = \tau_1^*.\ \tau_2^*$ and $\psi = \tau_1^* + \tau_2^*$. Taking the inverse transform

$$y(t) = \phi \ddot{v} + \psi \dot{v} + v$$

Consequently the state matrix C changes to

$y = [1 \ \psi \ \phi]\mathbf{x}$

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