

THERMOGENESIS: HARMONIC ANALYSIS AND UNIVERSAL TRANSFERENCE FUNCTION

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ABSTRACT

This work considers how the ratio signal/noise and the introduction of a cut-off frequency affect the calculus of the thermogenesis. In particular, the validity of the experimental criterion used to calculate this frequency inside the deconvolutive calculus is studied. The deconvolutive efficiency of the universal transference function is also presented comparatively.

INTRODUCTION

One of the approaches to the thermokinetic problem has been focussed on the transfer function (TF) of the calorimetric system calculated from experimental thermograms by means of the Fast Fourier Transform (FFT), laying aside, however, certain qualitative evaluations such as the effects introduced by the existence of noise in the experimental records or the techniques used to smooth the thermograms [1–5]. On the other hand, a universal transference function (UTF) vs. a reduced frequency scale has been recently proposed as a general representation for conduction calorimeters at low frequencies [6,7]. Consequently, this work presents the upper limits upon the transfer function introduced by the existence of experimental noise, an analysis of this cut-off frequency using the whole spectrum of the calorimeter, and the applicability of the UTF in the range of low frequencies.

EXPERIMENTAL NOISE

The existence of experimental noise (Johnson noise, electromagnetic perturbations, effects associated with the digital read-out system, etc.) forces us to introduce an upper limit to the spectrum of the calorimeter: ν_n . Should

we accept higher frequencies in the deconvolutive calculus, we would obtain a resultant thermogenesis considerably affected by noise. The experimental procedure led to the introduction ad hoc of ν_n in the TF given by [8]

$$\frac{|TF|_{\nu=\nu_n}}{|TF|_{\nu=0}} \approx \frac{\text{Amplitude of noise}}{\text{Maximum of the thermogram}}$$

The quantitative validity of the criterion has been tested up to now in two experimental systems: a BMR calorimeter [9] whose cell content is a high conductivity material, and the JLM-E1 calorimeter [10] — containing a poor conductor (silicone oil) in the laboratory cell — which is studied in this work (Fig. 1). This criterion is more restrictive than that used concerning linear systems: $|TF|_{\nu=\nu_n} \approx |\text{noise}|$.

The mathematical treatment has been based on an analytic representation of the experimental transfer function of the system consisting of a product of poles and zeros in the Fourier space. Provided that the calorimeter may be represented by a few exponential terms instead of the whole infinite series — at least within the range of low/intermediate frequencies — when the dissipation takes place in the symmetry axis, it is feasible to think in such an approximation although the second and other time constants appearing in the analytic expressions lack physical meaning [11]. For an axial dissipation the analytic approximation to the TF reads

$$TF(\omega) = S \frac{(i\tau^* \omega + 1)}{\prod_{i=1}^6 (i\tau_i \omega + 1)}$$

$\tau^* = -2.4 \text{ s}$	$\tau_1 = 183.5 \text{ s}$	$\tau_4 = 6.5 \text{ s}$
	$\tau_2 = 55.2 \text{ s}$	$\tau_5 = 2.5 \text{ s}$
	$\tau_3 = 12.3 \text{ s}$	$\tau_6 = 2.4 \text{ s}$

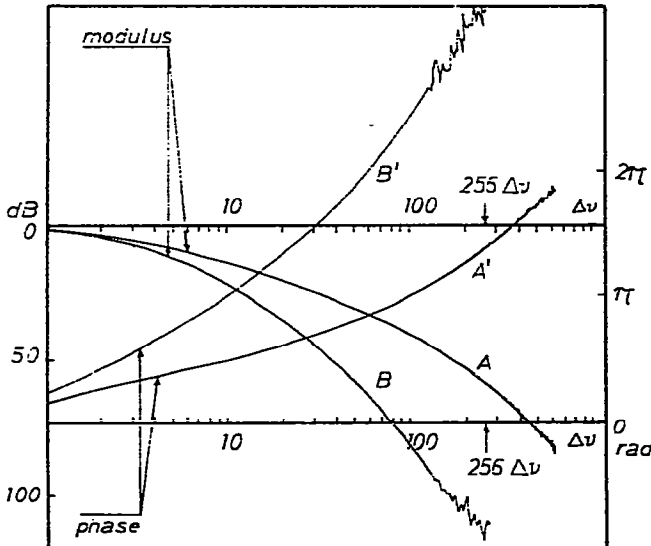


Fig. 1. Experimental TF of the JLM-E1 calorimeter calculated by means of the FFT. B and B' = an axial heat dissipation (measurement L88; $\nu_n \approx 0.07 \text{ Hz}$); A and A' = a dissipation near the detector system (L75; $\nu_n \approx 0.35 \text{ Hz}$).

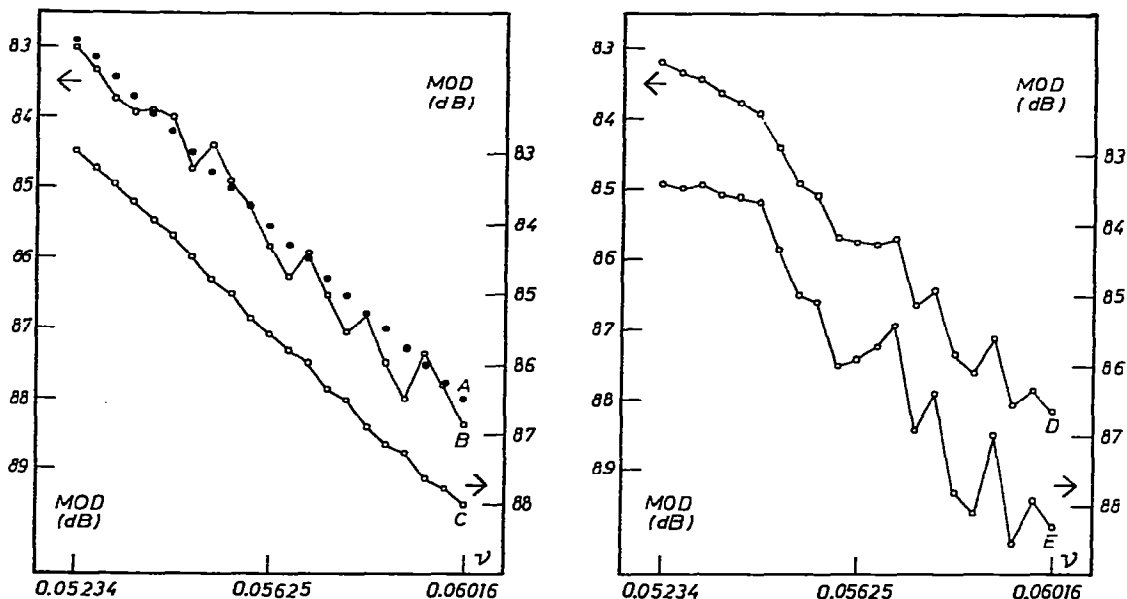


Fig. 2. Modulus in dB vs. frequency of: (A) mathematical model of the calorimeter; (B) experimental transfer function (m.: L82); (C) mathematical model plus a random noise whose noise/signal ratio is 5×10^{-6} ; (D) the same as (C) with noise/signal 2.5×10^{-5} (corresponds to the experimental noise/signal ratio); (E) the same as (C) and (D) with noise/signal 5×10^{-5} .

where S is the sensibility of the calorimeter in proper units (mV W^{-1} in our case).

Experimental noise has been simulated by a random routine in a Video Genie EG 3003 microcomputer. The amplitude of the noise thermogram is similar to the experimental noise (noise amplitude/maximum of the thermogram = 5×10^{-6} , $2.5 \times 10^{-5} \approx$ experimental noise, 5×10^{-5}).

The transform of the noise thermogram is obtained by means of the FFT and then added to the analytic transfer function given above (Fig. 2). In this way, we not only succeed in reproducing the experimental transfer function but we are also able to know quantitatively the oscillation of the TF at ν_n : ≈ 1 dB in all the amplitudes of the noise waveform studied.

CUT-OFF FREQUENCY ν_c

When calculating the thermogenesis using the FFT, the transform of the thermogram $F\{s(t)\}$ must be divided by the transfer function of the calorimeter TF. The thermogenesis is finally obtained by means of the inverse Fourier transform. Obviously the effects introduced by the existence of noise on the thermogram and the TF increase in an uncontrolled way with increasing frequencies, so the quotient between transforms yields arbitrarily large values for high frequencies which play a very important role in the integration to regain the thermogenesis.

Consequently one must define a cut-off frequency (a window) just to suppress high frequencies together with a technique capable of smoothing the

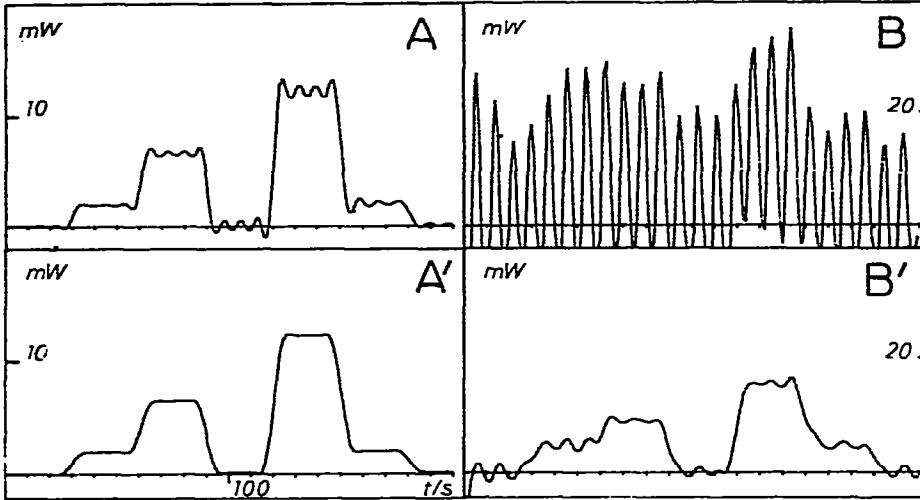


Fig. 3. Reconstructed thermogenesis using a cut-off frequency, $\nu_c = 256$, $\Delta\nu \approx 0.125$ Hz (the actual thermogenesis is shown in Fig. 4), for an axial dissipation (B). Smoothing the oscillation introduced in B by the cut-off frequency ν_c gives B'. A shows the reconstructed thermogenesis corresponding to a heat dissipation near the detector system. A' is A smoothed.

deformation introduced by such a window (see below). This frequency is strongly dependent on the relative position of the sources and the detector system, decreasing with the separation between them.

Figure 3 shows two calculated thermogenesis curves with $\nu_c = 256$, $\Delta\nu = 0.125$ Hz (Fig. 1), where $\nu_c > \nu_n$ in the axial dissipation (the thermogenesis obtained is clearly affected by noise) and $\nu_c < \nu_n$ in the coaxial dissipation, so giving quite an acceptable heat generation. The best performance is obtained when $\nu_c \approx \nu_n$.

Nevertheless, the use of a finite frequency spectrum introduces a perturbation on the thermogenesis which is on no account negligible and it is asymptotically a sinusoidal wave with decreasing amplitude for times far away from the generation of the signal.

Let us consider two examples.

(1) Rectangular pulse (used in calibration procedures) of width $(t_1 - t_0)$

$$f(t) = 0 \quad t_0 > t > t_1$$

$$f(t) = W \quad t_0 < t < t_1$$

The Fourier transform of this function is easily evaluated

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt = \frac{iW}{\omega} (e^{-i\omega t_1} - e^{-i\omega t_0})$$

Let us now introduce the finite inverse Fourier transform of $f(\omega)$, considering only that part of the spectrum between $(-\omega_c, \omega_c)$

$$f_{\omega_c}(t) = \frac{1}{2\pi} \int_{-\omega_c}^{\omega_c} \hat{f}(\omega) e^{i\omega t} d\omega$$

which after some calculus reduces to

$$f_{\omega_c}(t) = f(t) - \operatorname{Re} \left\{ \frac{W}{2\pi i} \left[\int_{t'\omega_c}^{\infty} \frac{1}{x} (e^{ix} - e^{-ix}) dx - \int_{t''\omega_c}^{\infty} \frac{1}{x} (e^{ix} - e^{-ix}) dx \right] \right\}$$

with $x = \omega t$, $t' = t - t_0$, $t'' = t - t_1$.

Finally, if we make use explicitly of the series expansion of $\operatorname{Si}(Z)$ [12] we can rewrite $f_{\omega_c}(t)$ as

$$\begin{aligned} f_{\omega_c}(t) &= f(t) - \frac{W}{\pi} \int_{t'\omega_c}^{t''\omega_c} \frac{\sin x}{x} dx \\ &= f(t) - \frac{W}{\pi} \left[\sum_n \frac{(-1)^n (t'\omega_c)^{2n+1}}{(2n+1)(2n+1)!} - \sum_n \frac{(-1)^n (t''\omega_c)^{2n+1}}{(2n+1)(2n+1)!} \right] \end{aligned}$$

Asymptotically $f_{\omega_c}(t)$ behaves as

$$\begin{aligned} f_{\omega_c}(t) &= f(t) - \frac{W}{\pi} \{ f(t'\omega_c) \cos(\omega_c t') + g(\omega_c t') \sin(\omega_c t') \\ &\quad - f(t''\omega_c) \cos(\omega_c t'') - g(\omega_c t'') \sin(\omega_c t'') \} \end{aligned}$$

where

$$f(z) \sim \frac{1}{z} (1 - 2!/z^2 + 4!/z^4 - \dots)$$

$$g(z) \sim \frac{1}{z^2} (1 - 3!/z^3 + 5!/z^5 - \dots)$$

(2) Sometimes the experimental thermogenesis is given by a series of exponential terms (first and higher order phenomena)

$$f(t) = 0 \quad t < 0$$

$$f(t) = \sum_{i=1}^N a_i e^{-\omega_i t} \quad t \geq 0 \quad (\omega_i > 0)$$

Similarly to the first example, we may calculate the finite inverse Fourier transform of the spectrum of the signal

$$f_{\omega_c}(t) = f(t) - \frac{1}{\pi} \sum_{i=1}^N a_i e^{-\omega_i t} \operatorname{Im}[E_1\{-(\omega_i + i\omega_c)t\}]$$

where the function $E_1(z)$ is defined by

$$E_1(z) = \int_z^{\infty} \frac{e^{-t}}{t} dt$$

It admits the following series expansion [12]

$$E_1(z) = -\gamma - \ln z - \sum_{n=1}^{\infty} \frac{(-1)^n z^n}{nn!}$$

where γ is Euler's constant.

Consequently

$$f_{\omega_c}(t) = f(t) + \frac{1}{\pi} \sum_{i=1}^N a_i e^{-\omega_i t} \left\{ \phi_i - \pi + \sum_{n=1}^{\infty} \frac{\rho_i^n \sin(n\phi_i)}{nn!} \right\}$$

where

$$z_i = \omega_i t + i\omega_c t = \rho_i e^{i\phi_i}$$

This expression can be well approximated when $\rho_i \gg 1$ by

$$f_{\omega_c}(t) = f(t) - \frac{1}{\pi} \sum_{i=1}^N a_i \left\{ \frac{1}{\rho_i} \sin(\omega_c t - \phi_i) + \frac{1}{\rho_i^2} \sin(\omega_c t - 2\phi_i) + \frac{2!}{\rho_i^3} \sin(\omega_c t - 3\phi_i) + \dots \right\}$$

showing an oscillatory behaviour when $\rho_i \gg 1$. This ripple can be eliminated by integration (smoothing) over a period: $T = 2\pi/\omega_c$.

Both examples lead to an extra oscillation on the thermogram of frequency ν_c , so justifying the smoothing technique which is usually applied on the thermogenesis obtained by finite deconvolution. Figure 3 (A \rightarrow A', B \rightarrow B') shows precisely the action of this smoothing technique when applied on the thermogenesis mentioned above. Figure 3B is associated with a cut-off frequency $\nu_c > \nu_n$, whereas in Fig. 3A $\nu_c < \nu_n$, and a remarkably correct thermogenesis is obtained.

DECONVOLUTION BY MEANS OF THE UTF

The introduction of a universal transfer function, UTF, allows enlargement of the range of frequencies attainable through a simple derivator with-

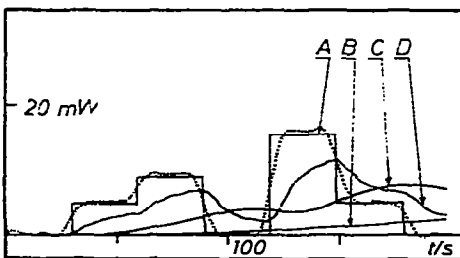


Fig. 4. A, Actual thermogenesis; B, the output thermogram; C, thermogenesis after the application of a one-step filter; D, deconvolution by means of the UTF. (.....) harmonic analysis.

out excessively increasing its complexity. Although the behaviour of the UTF is remarkably good within a range of frequencies which has been clearly established [7], it turns out to be necessary to evaluate its feasibility in a deconvolutive calculus applied directly on the temporal thermogram for, in this case, we make use of the whole spectrum of the thermogram.

Figure 4 presents comparatively the efficiencies of several deconvolutive techniques: harmonic analysis, a simple derivator and the universal transfer function. The structure of the UTF in Fourier space (product of three poles) leads to a three-step derivator on the thermogram. The derivation procedure follows the standard technique. The values of the poles are taken from ref. 7.

CONCLUSIONS

The criterion

$$\frac{|TF|_{\nu=\nu_n}}{|TF|_{\nu=0}} \simeq \frac{\text{Amplitude of noise}}{\text{Maximum of the thermogram}}$$

gives a suitable value for the maximum frequency attainable in the deconvolutive calculus ν_n , which arises from the experimental noise in the thermogram and the transfer function. A deconvolution including frequencies higher than that upper limit ν_n proves to be inadequate. Obviously, during the deconvolutive calculus it is of fundamental importance to obtain a transfer function with a high signal/noise ratio with respect to that of the thermogram.

The frequency ν_n , and consequently ν_c strongly depend on the relative position of the sources and the detector system, especially for very favourable noise/signal ratios (10^{-3} or less).

A finite inverse Fourier transform to yield the thermogenesis introduces a perturbation which is not at all negligible. This perturbation asymptotically reduces to a sinusoidal oscillation (whose frequency is precisely the maximum frequency used in the integration) with decreasing amplitude and can be conveniently suppressed by means of the usual integration technique over a period $T = 1/\nu_c$. This technique also allows smoothing of the influence of experimental noise when $\nu_c \simeq \nu_n$.

The universal transfer function exhibits deconvolutive characteristics clearly superior to a simple derivator without increasing the number of data required. Only information concerning the content of the laboratory cell needs to be added.

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