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# THERMOGENESIS: SMOOTHING TECHNIQUES IN Z-TRANSFORM AND HARMONIC ANALYSIS

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## ABSTRACT

This work analyses how the standard smoothing techniques affect the thermogenesis given by harmonic analysis or Z-transform methods. The analysis has allowed an optimization of their efficiency. The results concerning signal/noise ratios of 40, 60, 80 and 100 dB are tabulated and generalized to a reduced frequency representation.

## INTRODUCTION

In recent years, considerable effort has been devoted to devising fully working algorithms to yield the thermogenesis, namely harmonic analysis (based on the Fast Fourier Transform) [1], numeric [2] or analogic [3] inverse filters, dynamic optimization (conjugate gradient) [4], deconvolution by means of Z-transform [5] and, finally, methods based on optimal pursuit [6] or on a thermogram expansion in terms of an orthogonal set of rectangular pulse thermograms [7]. All of them have already been tested on different calorimeters and a great variety of heat dissipations, including thermogenesis corresponding to physical phenomena, have yielded really relevant results [8].

Nevertheless, the existence of experimental noise on the thermograms clearly handicaps the obtention of the thermogenesis. Furthermore, there may appear extra oscillations on the thermogenesis depending on the deconvolutive technique used to perform the calculations. This is the case, for instance, of harmonic analysis where the introduction of a window suppress-

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ing high frequencies itself takes an oscillation [9,10]. This window is essential in order to eliminate that part of the spectrum affected by the experimental noise. In a similar way it is also advisable to consider that window when performing inverse filtration [11].

On the other hand, a systematic analysis of the dynamic response of several calorimeters has led to the introduction of a relative representation both in time ($t/\tau_1$, where $\tau_1$ is the first time constant of the calorimeter) and frequency ($\nu\tau_1$) [12]. This representation shows the dynamic behaviour of different calorimeter groups around a certain half transfer function [12]. Consequently, any result concerning a given calorimeter may be readily generalized to this average behaviour provided such a relative representation is adopted, and since its signal/noise ratio is known the kinetic limits of a given calorimeter may be calculated [12].

In this work, we examine (taking for granted such a relative representation) whether the quality of the resultant thermogenesis is modified by the standard smoothing techniques used in inverse filtration or Z-transforms. We also analyze the integration over $T_c$ ($\nu_c = 1/T_c$, $\nu_c$ being the cutoff frequency in harmonic analysis) that partially suppresses the extra oscillation given by a finite inverse Fourier Transform. The different smoothing options are tabulated in a relative scale according to the signal/noise ratio of a given device.

## DECONVOLUTION BY HARMONIC ANALYSIS

The thermogenesis can be obtained from

$$e(t) = T^{-1}\,[\mathrm{TS}/\mathrm{TF}]$$

where $T^{-1}$ is the inverse Fourier transformation, TS is the Fourier Transform of the thermogram, and TF is the transfer function of the device. These transforms are performed with the aid of the Fast Fourier Transform algorithm (FFT).

Generally, the experimental noise which affects both the thermogram and the transfer function considerably deforms the thermogenesis if the deconvolution includes frequencies higher than a certain frequency $\nu_n$ which depends essentially on the signal/noise ratio. Therefore a cutoff frequency $\nu_c(\nu_c \lesssim \nu_n)$ must be introduced to suppress this part of the spectrum.

However, such a frequential window brings about an extra oscillation superimposed on the thermogenesis which is in no way negligible. Such an oscillation asymptotically reduces to a sinusoidal wave with decreasing amplitude and period $T_c = 1/\nu_c$ [9]. A simple integration over $T_c$ has been introduced as an easy way to partially eliminate it [9,10] although in the literature more sophisticated methods exist (see, e.g., Lanczos convergence factors in ref. 13).

The integration over $T_c$

$$\tilde{s}(t)=\frac{1}{T_c}\int_{t-T_c/2}^{t+T_c/2}s(t')\,dt'$$

is equivalent to applying an extra filter on s($t$) whose frequential representation is (see Appendix)

$$\tilde{s}(p)=\frac{1}{T_c}\,\frac{e^{pT_c/2}-e^{-pT_c/2}}{p}\,s(p)$$

Consequently, integrating the resultant thermogenesis gives rise to a modification in the dynamic gain of the system. This modification can be seen in Fig. 1 where the action of the filter is represented together with the transfer function of the JLM-E1 calorimeter. In fact, relative frequency representation clearly shows that the frequency range attainable by any conduction calorimeter is not actually much larger than that of the JLM-E1 calorimeter (see ref. 10), which is why the analysis has been focussed on the TF of this calorimeter corresponding to two different locations of the heat sources: on the axis of the calorimetric vessel (left) and near the detector system (right). $T_c$ is 8 s and 2 s, respectively (see ref. 9 for a full explanation of the choice of cutoff frequency and integration period). $\nu_c$ decreases with decreasing signal/noise ratios and, consequently, integration periods rise. An adequate choice of $T_c$ leads to a reduction in the influence of noise but

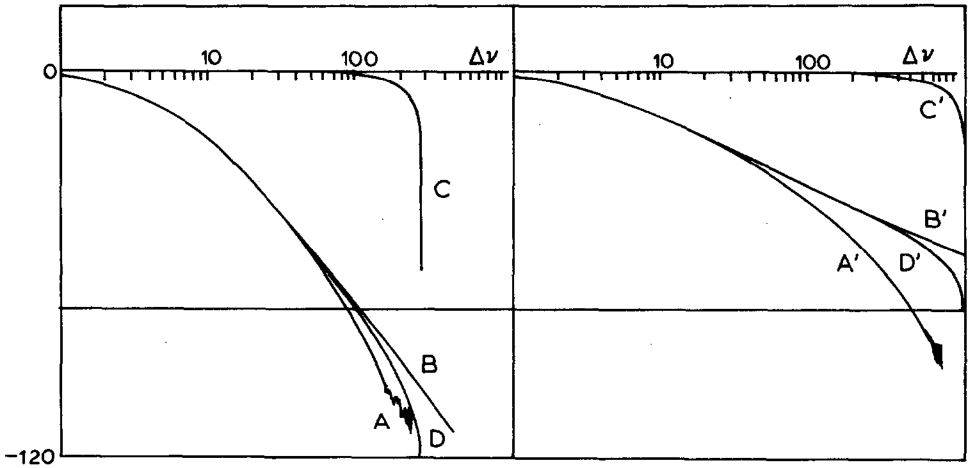


Fig. 1. Experimental transfer function (modulus in dB and phase in rad) of the JLM-E1 conduction calorimeter (A and A′). B and B′ are the analytic approximations to the TF; C and C′ are the frequential representations of the integral smoothing over $T_c$; D and D′ are the analytical models plus the corresponding filter. (Unprimed capital letters stand for dissipations far from the detector system whereas primed ones correspond to dissipations near the detectors). $\Delta\nu = 1/2048$ Hz.

without loss of information. In other words, smoothing should only deform that part of the spectrum affected by noise and, in any case, this deformation should never exceed the uncertainty due to the noise itself.

With regard to analytical approximations of the RF [2] that progressively diverge from the actual TF of the system (B and B′, Fig. 1), a smoothing technique may be introduced to cancel the effect of the corrector from that frequency where the nodal and TF appreciably diverge. Now, such a smoothing technique would not affect the quality of the resultant thermogenesis if the deformation which it introduces is of the same order of magnitude as the divergence between the model and the TF or, in other words, the smoothing should only deform that part of the spectrum that has no useful information.

## DECONVOLUTION BY MEANS OF Z-TRANSFORM

The use of the pulsed transfer function requires the introduction of Truxal's method of compensation. The compensating plant resides in fictitious zeros which make the system physically possible. These zeros are chosen in such a way that they also smooth the experimental noise without affecting the quality of the thermogenesis obtained. On the other hand, the TF of the calorimeter may be obtained from its pulsed response and the FFT. This TF serves as a test for the model introduced to perform the Z-transform and to evaluate the influence of the added zeros.

Figure 2 shows both the experimental TF and the corresponding model (three poles); it is also seen that the three extra zeros (1.02 s, see ref. 5) added to the model only modify the actual TF of the system for frequencies beyond $\nu_n$. Consequently, the quality of the resultant thermogenesis remains unaffected. The reasoning behind the choice of these zeros is just the same as the choice of $T_c$ which was explained in the previous section.

If the signal/noise ratio decreases, the value of the zeros $\tau^*$ increases and, consequently, counteracts the effect of those poles $\tau_1 \lesssim \tau^*$. This means that with increasing noise amplitude, the deconvolutive possibilities decrease. The TF of the calorimeter used to test experimentally the efficiency of the method lies inside the fluctuation interval of TF (see Fig. 3), so the results obtained may be immediately translated to a general case.

## REDUCED REPRESENTATION

Reduced scales ($t' = t/\tau_1$ and $\nu' = \nu\tau_1$) have been proposed to systematize the behaviour of different calorimeters. Figure 3 shows an average representation of the TF, $|TF(\omega)|$, together with the fluctuation range. Let us consider how the values of the compensating zeros of the pulsed transfer function and

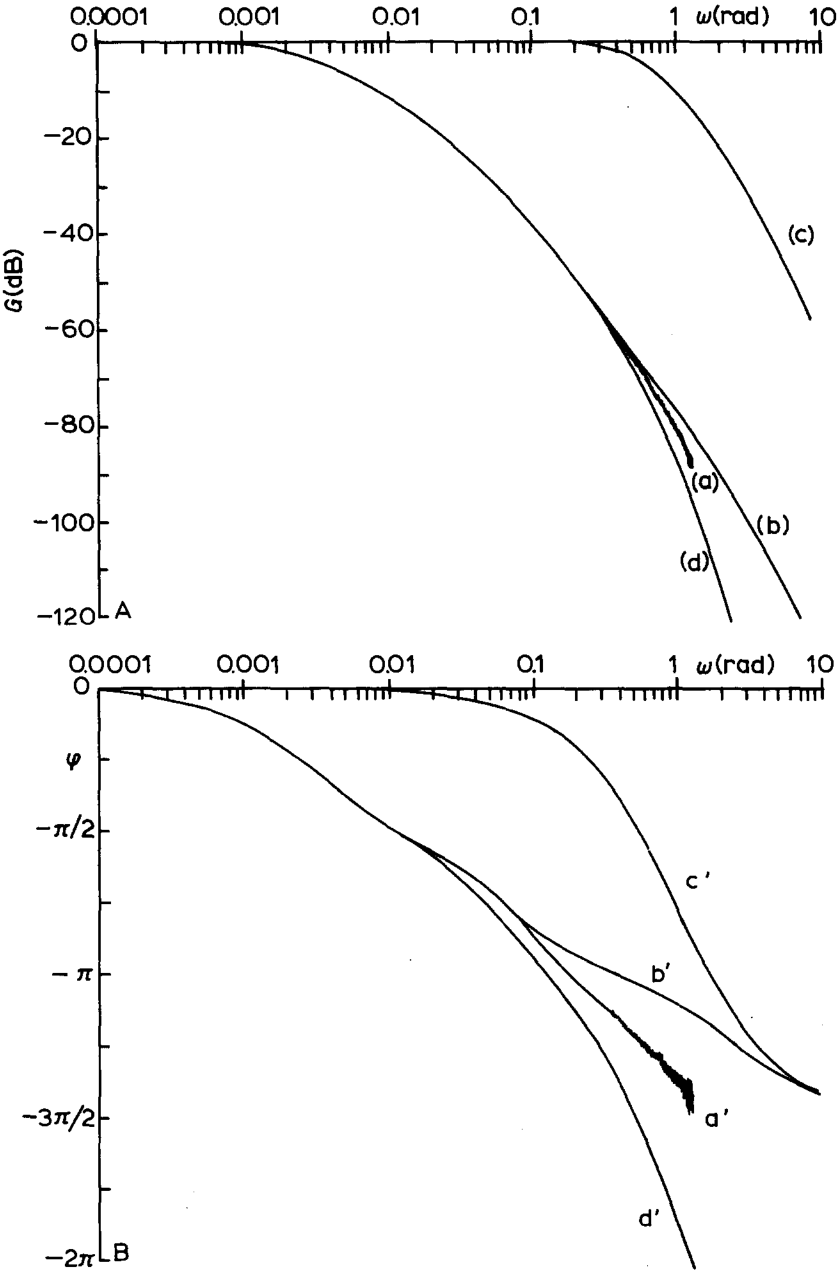


Fig. 2. Modulus (A) in dB and phase (B) in rad of: (a) experimental TF of STQ.ADA calorimeter; (b) model ($\tau_1 = 378.0$ s, $\tau_2 = 17.0$ s, $\tau_3 = 0.4$ s); (c) compensating plant (three poles $\tau^* = 1.02$); (d) model plus compensating plant.

also the values of $T_c$ used to smooth the thermogenesis given by harmonic analysis may be calculated from the signal/noise ratio on this scale.

The zeros should, at most, add to the TF the same uncertainty as the

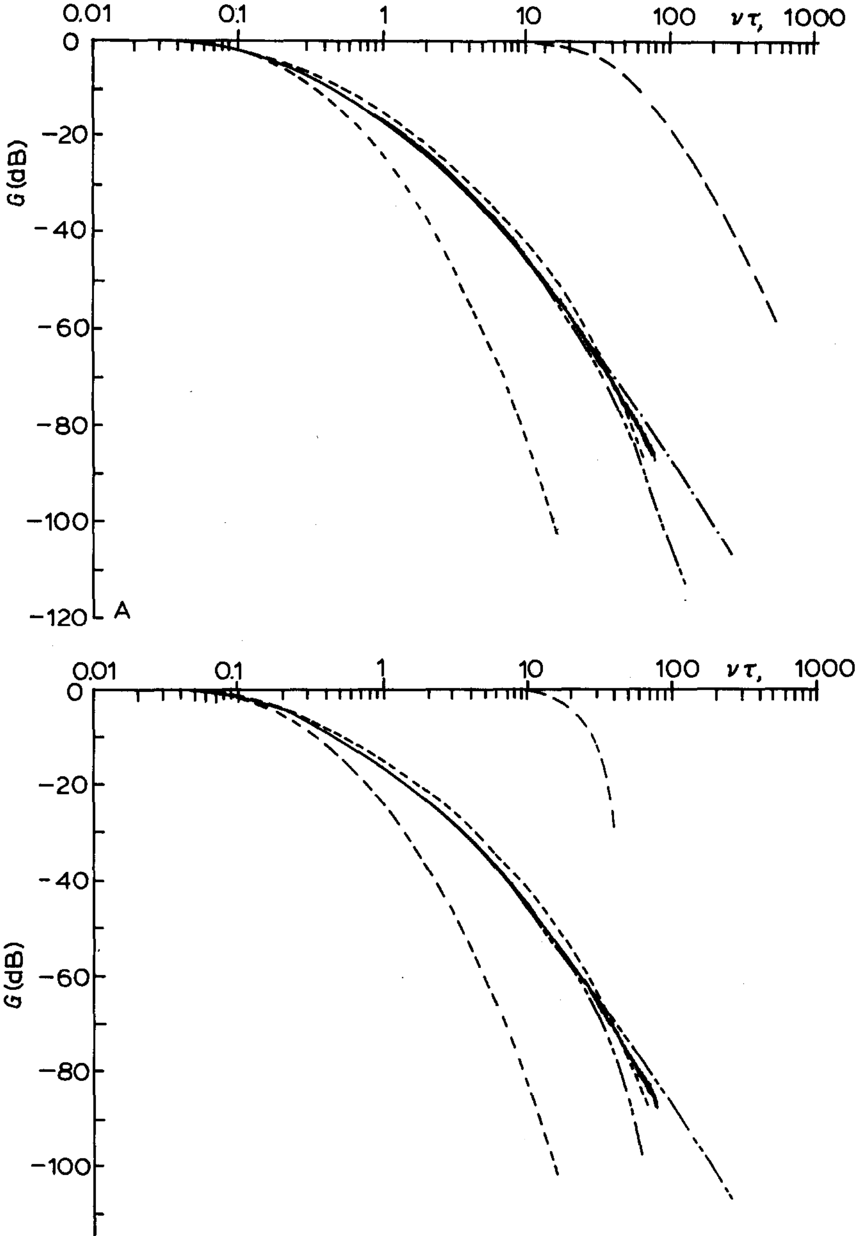


Fig. 3. The effect of the smoothing techniques discussed in the text. A is related to the Z-transform and B is related to harmonic analysis (both are presented in reduced units). (— — —) are two different locations of the sources in the JLM-E1 calorimeter. They show the widest range of variation on this scale. (———) is the experimental transfer function of the STQ-ADA calorimeter [5]. (·–·–·) is the analytical approximation to the experimental TF. (— —) represents the smoothing filters in reduced units proposed in the text, either the compensating plant (A) or the integration over $T_c$ (B). (··–··–) is the analytical model plus the corresponding filter (A or B).

TABLE 1

Selected values of the parameters defining both filters presented in the text in reduced units and for different signal/noise ratios $N_c^{min}$ and $N_c^{max}$ represent the lower and upper limits depending on the cell constants and the location of the sources in the case of harmonic analysis.

| S/N (dB) | $\overline{\nu\tau_1}$ | $\tau^*/\tau_1$ | $f$ | $\nu_c\tau_1$ | $N_o$ | $N_0^{min}$ | $N_0^{max}$ |
|---|---|---|---|---|---|---|---|
| 40 | 5 | 0.013 | 2 | 14 | 94 | | |
| 60 | 13 | 0.005 | 2.3 | 36 | 243 | 229 | 257 |
| 80 | 24 | 0.0027 | 2.4 | 66 | 449 | 411 | 513 |
| 100 | 45 | 0.0015 | 2.2 | 123 | 842 | 684 | 1025 |

noise. As a reference, this uncertainty is taken as 2 dB (see the Appendix). We then calculate the values of the zeros belonging to the compensating plant in reduced units and corresponding to various signal/noise ratios, and their range of fluctuation depending on the cell contents or the location of the heat sources [10].

The elimination of the extra oscillation caused by the cutoff frequency in harmonic analysis gives rise to a criterion very similar to the previous one. Now we look for a frequency, say $\nu_{2\,\mathrm{dB}}$, where the noise superimposed on the TF exceeds 2 dB. We than make the filter introduce, at most, the same deformation at the same frequency. This condition allows us to calculate the period $T_c$ of the filter and consequently the cutoff frequency which is to be used in the calculus: $\nu_c \cong 2.74\ \nu_{2\ \mathrm{dB}}$ (see the Appendix and Table 1). In this way the deformation introduced by the filter never exceeds the uncertainty brought about by noise. However, due to the fact that the FFT handles a set of $N$ points where $N = 2^M$ ($M$ is an integer), the choice of $\nu_c$ is not arbitrary (see Table 1 in ref. 10). Table 1 shows the values of $\nu_c$ in terms of the equivalent frequency intervals $N_c[\nu_c = (N_c - 1)\Delta\nu]$. It should also be remembered that the standard sampling period is $\Delta t \simeq \tau_1/300$ since this period allows an adequate representation of the system's dynamic response up to signal/noise ratios $\simeq 10^5$ (100 dB).

## CONCLUSIONS

When the deconvolution is performed by means of Z-transforms a certain number of extra zeros must be added to the model for the TF so that the number of poles is the same as the number of zeros. The values of the extra zeros, in reduced units, should be $\tau^*/\tau_1 = 0.065/(\nu_n\tau)$. $\nu_n$ is the frequency where the experimental noise on the TF amounts to 2 dB. If the deconvolution were performed through harmonic analysis, the cutoff frequency would be given by

$$(\nu_c\tau_1) \simeq 2.74(\nu_n\tau_1)$$

Due to the average characteristics of calorimetric devices the previous criteria can be modified according to different amounts of noise. In fact, considering divergences ranging between 2 and 10 dB does not appreciably change the final result, neither the compensating zeros nor $T_c$. For instance, if $\nu_n$ corresponds to noise oscillations ranging around 10 dB then, similar calculations yield

$$\tau^*/\tau_1 \simeq 0.17/(\nu_n\tau_1)$$

and correspondingly

$$(\nu_c\tau_1) \simeq 1.36(\nu_n\tau_1)$$

Harmonic analysis deals with a discrete frequency spectrum. If an easy suppression of the ripple is intended then $N_c = N/(n+1)$ where $n$ is an integer, $N = 2^M$ is the number of points handled by the routine, and $\nu_c = (N_c - 1)\Delta\nu$. Now if one finds a 2 dB (10 dB) fluctuation at $N_n$, $N_c$ should be the nearest integer to 2.74 $N_n$ (1.36 $N_n$).

## REMARK

We have only been dealing with noise affecting the TF of the system. Consequently, integration and frequential limits given throughout the paper correspond to the most favourable situation, i.e., the frequential limits given should be reduced if the signal/noise ratio of the thermogram is lower than that of the TF.

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## APPENDIX

A. A Simple way to partially suppress the ripple on the thermogenesis caused by a finite inverse transform is

$$\tilde{f}(t)=\frac{1}{T_c}\int_{t-T_c/2}^{t+T_c/2}f(t')dt'$$

Taking the derivative of this expression

$$\tilde{f}'(t)=\frac{1}{T_c}[f(t+T_c/2)-f(t-T_c/2)]$$

The Laplace Transform of $\tilde{f}'(t)$ now yields

$$s\,\tilde{F}(p)-\tilde{f}(0)=\frac{1}{T_c}\left[\int_0^{\infty}f(u)e^{-p(u-T_c/2)}du-\int_0^{\infty}f(r)e^{-p(r+T_c/2)}dr\right]$$

$$=\frac{1}{T_c}[e^{pT_c/2}-e^{-pT_c/2}]F(s)$$

Taking $\tilde{f}(0)=0$, then

$$\tilde{F}(p)=\frac{1}{T_c}\frac{e^{+pT_c/2}-e^{-pT_c/2}}{p}F(p)$$

Its phase is zero and its modulus is

$$|\tilde{F}(\omega)|=\left|\frac{\sin(\omega T_c/2)}{\omega T_c/2}\right||F(\omega)|$$

Let us now consider a divergence between $|\tilde{F}(\omega)|$ and $|F(\omega)|$ of 2 dB, then

$$2=20\log\left|\frac{\sin(\omega_{2\,dB}T_c/2)}{\omega_{2\,dB}T_c/2}\right|\qquad(\omega_{2\,dB}=2\pi\nu_{2\,dB};\ \nu_c=2\pi/T_c)$$

Solving for $\nu_c$: $\nu_c=2.74\ \nu_{2dB}$. (If the divergence 10 dB, then $\nu_c=1.36\ \nu_{10\,dB}$.)
B. Smoothing through a triple zero considers a compensating plant which reads

$$G(s)=(1+\tau^*s)^3$$

whose modulus (dB) and phase (rad) are

$$G(\nu)=20\log(1+4\pi^2\nu^2\tau^{*2})^{3/2}$$

$$\psi(\nu)=3\tan^{-1}(2\pi\nu\tau^*)$$

Considering again a divergence of 2 dB, we obtain

$$2=30\log(1+4\pi^2\nu_{2\,dB}^2\tau^{*2})$$

Finally

$$\tau^*=0.065/\nu_{2\,dB}$$

Correspondingly

$$\tau^*=0.17/\nu_{10\,dB}$$