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THERMOGENESIS: IDENTIFICATION BY MEANS OF MODULATING FUNCTIONS

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ABSTRACT

This paper describes how to obtain an analytic approximation to the transfer function of a conduction calorimeter, namely a procedure to identify the calorimetric system. In this case modulating functions are used directly on the thermogram. The method is used twice: to obtain the time constants and the amplitudes. Its feasibility is tested on two models which span the frequency range usually attained by actual calorimeters. The influence of random noise and baseline drift have also been analyzed. The results show that three or four time constants are correctly obtained.

INTRODUCTION

This work, a continuation of that described in ref. 1, presents an identification method based on modulating functions. The method allows an analytic approximation to the transfer function of a heat flux calorimeter. Its performance has been tested on the same analytic models used in ref. 1.

APPROXIMATION USING MODULATING FUNCTIONS. ALGORITHM

The pulsed response of a heat flux calorimeter may be well approximated by a finite series

$$s(t) = \sum_{i=1}^{N} a_i \exp(-t/\tau_i)$$

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which may be regarded as the solution to a differential equation

$$s(t)+A_1\dot{s}(t)+\ldots+A_N s^{(N)}(t)=0$$

where the coefficients $A_1,\ldots,A_N$ are functions of the time constants of the system

$$A_1=\sum_{i=1}^{N}\tau_i,\ A_2=\sum_{1=i<j}^{N}\tau_i\tau_j,\ldots,A_N=\prod_{i=1}^{N}\tau_i$$

Once the pulsed response is known, the identification of the system is carried out by determining the coefficients $A_1,\ldots,A_N$ which define the differential equation. The obvious way is to derive numerically $s(t)N$ times in N different times, thus obtaining a system of linear equations which can be solved immediately. Nevertheless, $s(t)$ is a sampled function affected also by random components so the noise waveform is considerably amplified after each derivative. What is more, high frequencies are cut off because of the derivation step required by high order derivatives.

The modulating function method (MFM) offers an alternative way of facing the problem. This method is a general technique to obtain the coefficients of a linear differential equation [2]. A modulating function (MF) of order N is defined as any function $\varphi(t)$ well behaved inside $[0,T]$ which verifies $\varphi(t)=\varphi'(T)=\ldots=\varphi^{(N+1)}(t)=0$ for $t=0$ and $t=T$.

A useful choice for our purposes is found to be [3]

$$\varphi(t)=t^n(T-t)^p$$

where n, $p>N$. If we multiply the differential equation by $\varphi(t)$ and integrate over $(0,T)$ we obtain

$$\int_0^T\varphi s\,\mathrm{d}t+\int_0^T A_1\varphi\dot{s}\,\mathrm{d}t+\ldots+\int_0^T A_N\varphi s^{(N)}\,\mathrm{d}t=0$$

The integrals containing derivatives of $s(t)$ may be integrated successively by parts in such a way that the derivatives are charged on the MF. We obtain

$$A_1[\varphi s]_0^T,\ -A_2[\varphi\dot{s}]_0^T,\ldots$$

which are zero because of the very definition of MF. Finally, the equation reduces to

$$\int_0^T\varphi s\,\mathrm{d}t-A_1\int_0^T\dot{\varphi}s\,\mathrm{d}t+A_2\int_0^T\ddot{\varphi}s\,\mathrm{d}t-\ldots+(-1)^{(N+1)}A_N\int_0^T\varphi^{(N)}s\,\mathrm{d}t=0$$

The calculations may now be carried out with N different MF (different values of p and n), thus obtaining a system of linear equations whose solution is the set of N coefficients A_i. The time constants are now found to be the roots of

$$\tau^N-A_1\tau^{(N-1)}+A_2\tau^{(N-2)}+\ldots+(-1)^{(N)}A_N=0$$

Note how the algorithm does not require the calculus of the successive derivatives of s(t), thus not leading to a noise amplification [the derivatives of $\varphi(t)$ may be calculated analytically]. The MF and their derivatives behave as weight functions in the integrals of s(t) (Fig. 1). On the other hand, the

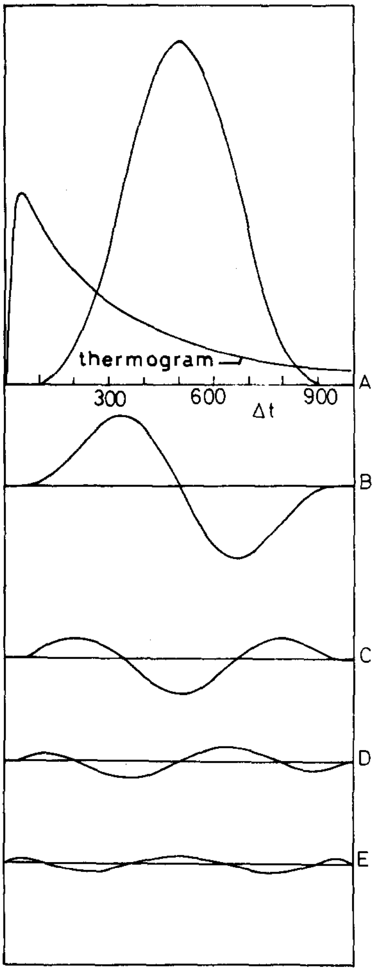

Fig. 1. Characteristic shape of an MF with $n = 5$, $p = 5$ (A) and its successive derivatives (B, C, D, E). The thermogram of model M9 is also shown but re-scaled by a factor of 10^{-5}. The sampling period of the thermogram is $\Delta t = 0.5$ s, whereas the Δt used to calculate the MF is 0.1 s.

integrals performed somewhat smoothen the noise present in the thermogram. Another advantage of the method is that it only requires a part of the thermogram and, in principle, its accuracy is not modified. This allows suppression of that part of the experimental thermogram which is considerably affected by noise, i.e. those intervals where the signal/noise ratio is especially low.

Once the time constants of the system have been calculated using this method, the corresponding amplitudes could be obtained using a least-squares approximation. The calculations performed clearly show that it is more convenient to use again the MF. We are now led to the following system of equations

$$\sum_{i=1}^{N} a_i \int_0^T \varphi_j \, e^{-t/\tau_i} \, dt = \int_0^T \varphi_j s \, dt \qquad (j = 1, \ldots, N)$$

where φ_j are different MF chosen following the criterion previously given.

RESULTS

In order to analyze the feasibility of the method we have used the same analytic models described in ref. 1:

M8		M9	
τ_i	a_i	τ_i	a_i
192.0	0.4866×10^6	192.0	0.2957×10^6
49.0	-0.7895×10^6	49.0	0.1577×10^6
18.0	0.3254×10^6	9.0	-0.3407×10^6
4.0	-0.2805×10^5	4.0	-0.2945×10^6
2.0	0.6227×10^4	1.2	0.2197×10^6
1.2	-0.7310×10^3	0.4	-0.5979×10^5
0.4	0.3281×10^1	0.3	0.2193×10^5
0.3	-0.4715×10^0		
$s(t)_{\max} = 192680.0$		$s(t)_{\max} = 333571.0$	

Their sensibility is $S = \sum_{i=1}^{N} a_i \tau_i = 0.605 \times 10^8$ in arbitrary units. The models roughly simulate the transfer function—corresponding to two different locations of the heat sources—of the calorimeter JLM-E1 [1]. In this case the thermogram units would be nV. Random noise and baseline drift have also been added to both models in order to reproduce better the usual experimental conditions. The various models are denoted as:

M8 (resp. M9) + 50 N: random noise ranging ±50 units (signal/noise ≃ 70 dB);

M8 (resp. M9) + 50 D: linear drift where the last ordinate is shifted by + 50 units;

M8 (resp. M9) + 50 N + 50 D: random noise plus base line drift.

The first point to be considered is the order of the transfer function which will be approximated to the given models. We have used in what follows a four-order approximation because we feel that this order will be adequate for

TABLE 1

Results given by the MFM concerning model M8 and its variants

M8		M8 + 50 N		M8 + 50 D		M8 + 50N + 50D	
192.00	0.4866E + 06	192.01	0.4865E + 06	191.95	0.4868E + 06	191.96	0.4867E + 06
49.00	−0.7895E + 06	48.97	−0.7903E + 06	49.05	−0.7879E + 06	49.02	−0.7887E + 06
17.99	0.3261E + 06	18.05	0.3256E + 06	17.77	0.3309E + 06	17.83	0.3298E + 06
4.40	−0.2562E + 05	3.99	−0.2158E + 05	6.92	−0.2518E + 05	6.73	−0.2114E + 05

TABLE 2

Results given by the MFM concerning model M9 and its variants
The last two files give the corresponding zeros calculated from the time constants and amplitudes obtained.

M9		M9 + 50 N		M9 + 50 D		M9 + 50N + 50D	
192.00	0.2957E + 06	192.02	0.2956E + 06	191.91	0.2959E + 06	191.94	0.2958E + 06
48.99	0.1577E + 06	49.11	0.1572E + 06	48.82	0.1584E + 06	48.95	0.1578E + 06
9.22	−0.2966E + 06	8.59	−0.4001E + 06	11.28	−0.1160E + 06	10.02	−0.2005E + 06
5.02	−0.2593E + 06	3.46	−0.1767E + 06	6.51	−0.4234E + 06	5.98	−0.3388E + 06
	63.97		64.08		63.80		63.92
	6.89		4.85		10.23		8.49

TABLE 3

Change in the time constants identified in models M8 and M9 with increasing the order of the approximation

The Table shows that the sampling period of the thermogram ($\Delta t = 0.5$ s) is a lower bound for the $\{\tau_i\}$ which may be properly identified. The best accuracy is obtained when the order in the approximation coincides with the number of positive real τ_i obtained ($M = 6$ in our case). The main time constants remain unchanged with increasing order and their values converge to the values of the model.

τ_i	M						
	5		6		7		8
	a_i	τ_i	a_i	τ_i	a_i	τ_i	a_i
Model M8							
192.00	0.4866 E06	192.00	0.4866 E06	192.00	0.4866 E06	192.00	0.4866 E06
49.00	−0.7894 E06	49.00	−0.7895 E06	49.00	−0.7895 E06	49.00	−0.7895 E06
17.99	0.3255 E06	18.00	0.3256 E06	18.00	0.3255 E06	18.00	0.3255 E06
4.18	−0.2550 E05	4.00	−0.3525 E06	3.94	−0.3105 E05	4.02	−0.2970 E05
0.20	0.5187 E05	2.02	0.3951 E05	2.42	0.9043 E04	1.96	0.1542 E05
		0.17	−0.7929 E06			0.02	−0.2113 E14
Model M9							
192.00	0.2957 E06	192.00	0.2957 E06	192.00	0.2957 E06	192.00	0.2957 E06
48.98	0.1577 E06	49.00	0.1577 E06	49.00	0.1577 E06	49.00	0.1577 E06
9.03	−0.3359 E06	9.00	−0.3409 E06	9.00	−0.3411 E06	9.00	−0.3407 E06
4.15	−0.2808 E06	4.00	−0.2917 E06	4.00	−0.2937 E06	4.00	−0.2946 E06
0.96	0.2084 E06	1.19	0.1749 E06	1.24	0.1966 E06	1.21	0.2166 E06
		0.50	0.6598 E05			0.17	−0.2266 E06

the identification of actual calorimetric systems. Experimental limitations (noise) bring about an upper bound for the attainable spectrum of the calorimeter, so a low order model may well approximate the transfer function within this limited frequency domain. All models have been reduced to unit surface and the sampling period selected has been $\Delta t = 0.5$ s. Previous tests have shown that the value of T selected does not affect the accuracy of the results provided that $T > 2\tau_i$. It should also be pointed out here that the sampling period selected represents, in fact, a lower bound for

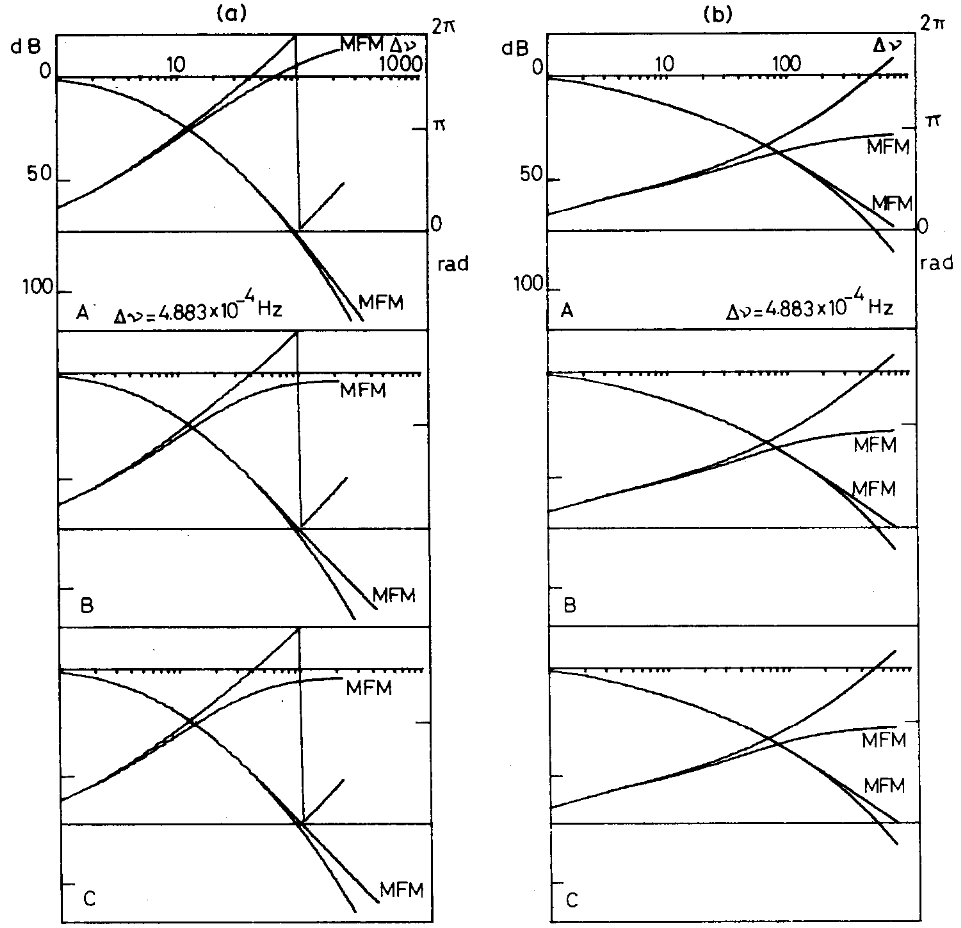

Fig. 2. Transfer functions of models (a) M8 and (b) M9 together with A, transfer function of the approximation given by the MFM algorithm (MFM) to models M8 + 50 N (a) and M9 + 50 N (b); B, transfer function of the approximation given by the MFM algorithm (MFM) to models M8 + 50 D (a) and M9 + 50 D (b); C, transfer function of the approximation given by the MFM algorithm (MFM) to models M8 + 50 N + 50 D (a) and M9 + 50 N + 50 D (b). The time constants and their corresponding amplitudes which define the approximation are given in Tables 1 and 2.

the time constants that can be identified. The MF actually used are defined by

n	5	5	5	6
p	5	7	9	5

concerning the calculus of the time constants, and by

n	1	2	5	7
p	5	5	5	5

concerning the amplitudes. In the latter case the integration step is 5 Δt which is enough for all the present purposes saving, on the other hand, computer time. The time scale has been re-scaled by a factor of $1/5$ to avoid an uncontrolled increase in the MF. Moreover, the MF have been divided in actual calculations by 10^{16}. The results obtained are presented in Tables 1 and 2.

The results show that the present version of the method gives, at least, three significant time constants and their corresponding amplitudes. Moreover, the selection of the model order is not especially critical insomuch as the larger time constants do not change when the order of the approximation is increased. However, concerning more complex systems, approximating a higher order model is strongly recommended for it ensures the correctness of the larger time constants. Note how in Tables 1 and 2 the fourth time constant is wrong (there is up to a 30% error) because this time constant must include in our fourth order model the contribution arising from the lower ones. After having increased the order of the approximation, at the cost of more computing time, the value of the fourth time constant improves (Table 3).

Finally, Fig. 2 shows, for both models and their corresponding modifications, their frequency spectra together with the approximations given by the MFM.

CONCLUSIONS

Details of the calculations can be summarized as follows: double precision —16 digits—has been used throughout the routine. T has been taken to be 500 s which means taking 1000 points of the thermogram because the actual sampling period is $\Delta t = 0.5$ s. During the calculations the time scale is divided by five and the thermogram surface is set equal to one. The MF are divided by 10^{16} to avoid excessive growth in their numeric values. In our case $T \approx 4\tau_1$.

The algorithm presented based on modulating functions gives in a systematic way the more relevant exponential terms in the development of s(t). The method uses the sampled pulse response of the system together with the order of the model to be approximated, which has to be fixed in advance.

In a similar fashion to that reported in ref. 1, the method gives an approximation to the transfer function not especially sensitive to the perturbations introduced and it is an adequate representation of the transfer function within the frequency domain usually attainable in actual calorimeters. (The signal/noise ratio is the same as that used previously: 70 dB [1]).

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