Thermochimica Acta, 89 (1985) 315–324
Elsevier Science Publishers B.V., Amsterdam – Printed in The Netherlands

THERMOGENESIS: COMPARATIVE STUDY OF SEVERAL DECONVOLUTION METHODS IN TIME-INVARIANT CALORIMETRY

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(Received 22 January 1985)

ABSTRACT

A comparative analysis of the performance of different deconvolution methods is presented. This includes harmonic analysis (HA), inverse filtering (IF), dynamic optimization (DO), optimal control (OC) and Z-transform (ZT). The methods are applied on simulated thermograms corresponding to time-invariant representative models of heat conduction calorimeters. The results suggest that: (1) IF and ZT are the simplest methods and give the best reconstructions of the heat power; (2) HA spends more computing time and memory space to achieve a similar quality in the thermogenesis; and (3) DO and OC, with the same expense in memory and time as HA, give much more inaccurate results when the power dissipation lasts a long time. On the other hand, it should be noted that to the present, IF and, conceptually, ZT and OC may be generalized to time-varying calorimetry.

INTRODUCTION

On one side, the dynamic characteristics from a great deal of different heat flux calorimeters have been systematically studied in recent years. After this study it follows that the kinetic performance of a certain device (i.e., its frequential limitations) may be established directly from its first time constant and the signal-to-noise ratio present in the measurement. Additionally, multi-body models, which qualitatively represent the behaviour of several calorimetric devices, have also been designed.

On the other side, to the present, quite a lot of different deconvolution methods in time-invariant calorimetry have been proposed and tested. We may mention harmonic analysis [1], dynamic optimization [2], inverse filtering [3], tracking based on optimal control [4], Z-transform methods [5] and the explicit inversion of the heat transport equations defining an RC model of the calorimetric system [6].

0040-6031/85/$03.30

These deconvolution methods have generally been tested on the Joule effect measurements, either comparing the resulting thermogenesis from the different algorithms, or comparing directly with the input heat power which is well known.

In this work we make a comparative analysis of the dynamic performance of the different methods by using numerical models and the corresponding simulated thermograms, and by computing the results obtained in frequency space. The analysis is meaningful if the methods tested are to be applied, as they usually are, in low-cost personal computers whose typical memory space is 64 kb. We also compare the computing time and memory space occupation of the different methods.

MODELS AND METHODS

First we have simulated two different calorimetric impulse responses which correspond roughly to the axial and external dissipations in the JLM-E-2 calorimeter [7]. These impulse responses have been shown to cover, in a reduced frequency scale (see, for instance, Fig. 1 and ref. 8), practically the whole frequency range usually attainable in heat flux calorimetry. In Laplace space the dynamic behaviour of a calorimeter is given by its transfer function, TF, which, in a general form, reads

$$\mathrm{TF}(p) = S\frac{\prod_{j=1}^{M}(\tau_j^* p + 1)}{\prod_{i=1}^{N}(\tau_i p + 1)}$$

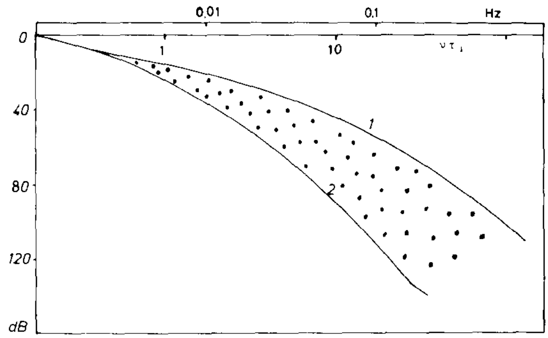

Fig. 1. Modulus (dB) vs. frequency (absolute (Hz) and relative scale ($\nu\tau_1$)) for the transfer functions corresponding to the models M8 and M9. (1) Systems of high thermal conductivity materials in calorimetric vessel (model M9 from ref. 7). (2) Systems with lower thermal conductivity (model M8). The transfer functions for different calorimeters stand in the dotted domain.

TABLE 1

Values of τ_i and τ_j^* defining the models M8 and M9

M8	τ_i	192	49	18	–	4	2	1.2	0.4	0.3
M9	τ_i	192	49	–	9	4	–	1.2	0.4	0.3
	τ_j^*	64	6							

We will call M8 the thermogram with the slowest descent, which corresponds to the axial dissipation, and M9 the thermogram of the peripheral dissipation. The corresponding values for their poles and zeros are given in Table 1. As we will refer to a relative gain scale in dB, we may take the static gain $S = 1$. In practice the static gain of the JLM-E-2 is approximately 0.605E08 nV/W.

As a test for comparison we have numerically performed the convolutions of the heat power input in Fig. 2 with the two models, and obtained the corresponding simulated thermograms. The heat power input has been chosen in accordance with that used in real Joule effect measurements in refs. 3 and 7. The thermograms have been sampled at intervals of $\Delta t = 0.5$ s, which gives a frequency spectrum wide enough (upper limit is the Nyquist frequency $1/(2\Delta t)$) to make the dynamic gain change by more than 100 dB. This is clearly more than what can be expected in a calorimetric system.

In all the following deconvolutions, the proper TF, i.e., the TF of the model used to perform the convolution, has been considered. However, every method makes explicit use of the transfer function in a different way. In some cases the values of poles and zeros of the model are necessary, while in others the deconvolution method requires the whole TF in time or frequency space.

The way in which the analysis has been carried out may be summarized as follows: for each deconvolution method, the Fast Fourier Transforms of the input signal (in Fig. 2) and of the thermogenesis achieved have been

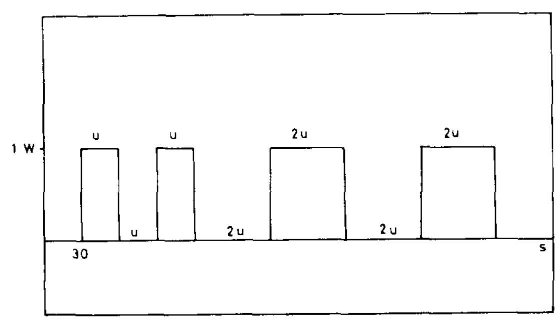

Fig. 2. Simulated heat power input from which the thermograms used in the deconvolutions have been calculated. In the present analysis $u = 32$ s.

calculated. The quotient between these two transforms determines the degree of performance in obtaining the thermogenesis at each frequency. A perfect deconvolution would yield a value of one at all the frequencies for this quotient of modulus.

Different trials have been carried out with each method attempting to optimize the results. The influence of the electric noise present in the measurement, and of the different modifiable parameters in each method, have been particularly analysed.

Inverse filtering (IF)

The thermogenesis is obtained by a stepwise elimination of the poles and zeros in the TF. Numerically, the filtering is performed by equations of

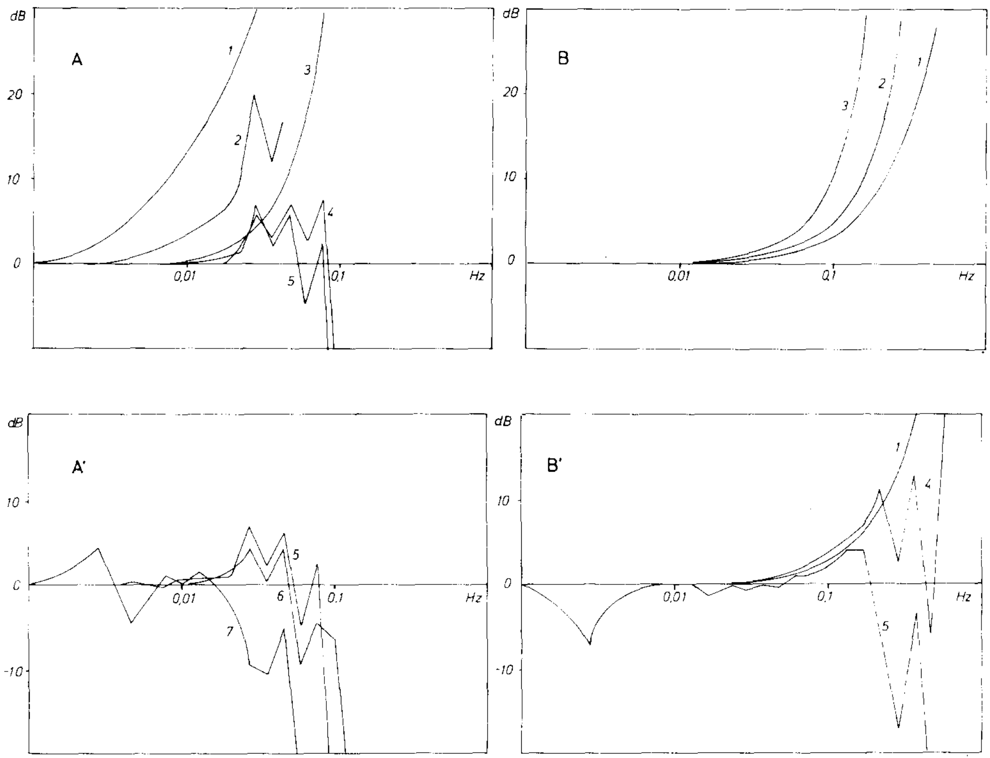

Fig. 3. (A), (A′) Results of inverse filtering (IF) for the transfer function M8. (1) Filtering the first pole with a time step of 1 s in the derivative. (2) Two poles and a time step of 2 s. (3) Three poles and a time step of 4 s. (4) Three poles and a time step of 2 s. (5) Three poles and a time step of 1 s. In all the cases above, the signal/noise ratio is 140 dB. (6) Three poles and a time step of 1 s, with s/n = 80 dB. (7) Three poles and a time step of 1 s, with s/n = 60 dB. (B), (B′) Results of filtering (IF) 4 poles and 2 zeros from M9, with different time steps in the numerical derivatives. (1) $K\Delta t = 0.5$ s; (2) $K\Delta t = 1$ s; (3) $K\Delta t = 2$ s; (4) $K\Delta t = 0.5$ s and signal/noise = 100 dB; (5) $K\Delta t = 0.5$ s and signal/noise = 80 dB.

differences of the form

$$s^+(I) = s(I) + \tau_i \frac{s(I+K) - s(I-K)}{2K\Delta t}\ ;\ s^+(I) = \frac{K\Delta t s(I) + \tau_j^* s^+(I-K)}{K\Delta t + \tau_j^*}$$

to eliminate the poles, $-1/\tau_i$, and to eliminate the zeros, $-1/\tau_j^*$. In these expressions the function searched for is $s^+(I)$, where I stands for the time of the measurement.

Figure 3 shows the results obtained by IF for both transfer functions. The different curves are obtained by changing the step K in the numeric derivatives above, and by using different levels of simulated noise on the thermogram. The noise is obtained from RANDOM computer routines and may be considered a white noise with a flat spectrum.

Z-transform (ZT)

The deconvolution based on the Z-transform may be seen as the generalization of inverse filtering to the case in which the use of digital systems leads to a discretization in the thermogram with a sample every Δt.

For the calculation to be convergent the transfer function has to be completed with a compensating plant leading to the same number of zeros and poles. It has been proposed [9] that the additional zeros may be calculated from the values of the frequencies where the noise in the TF becomes important. Figure 4 shows the results obtained with ZT.

Harmonic analysis (HA)

The harmonic analysis is based on the fact that the convolution product is an ordinary product in the Fourier space. Fourier transforms of the thermogram and the impulse response can be easily obtained by means of the Fast Fourier Transform. The quality in the results of deconvolution with HA mainly depends on two things: the frequential cut-off selected and the way in which the associated ripple is smoothed. In the present calculations we choose different cut-off frequencies, depending on the level of noise superimposed on the thermogram, in accordance with the criteria established in refs. 3 and 9. The results are shown in Fig. 5.

Dynamic optimization (DO)

The transfer function for performing a dynamic optimization must be in the form of an impulse response. A convolution between this response and a first approach to the thermogenesis gives a calculated thermogram. It must be compared with the experimental thermogram and, by means of a gradient search, approximated to it in an iterative way. At the last step, the input coupled with the best calculated thermogram is supposed to be the real

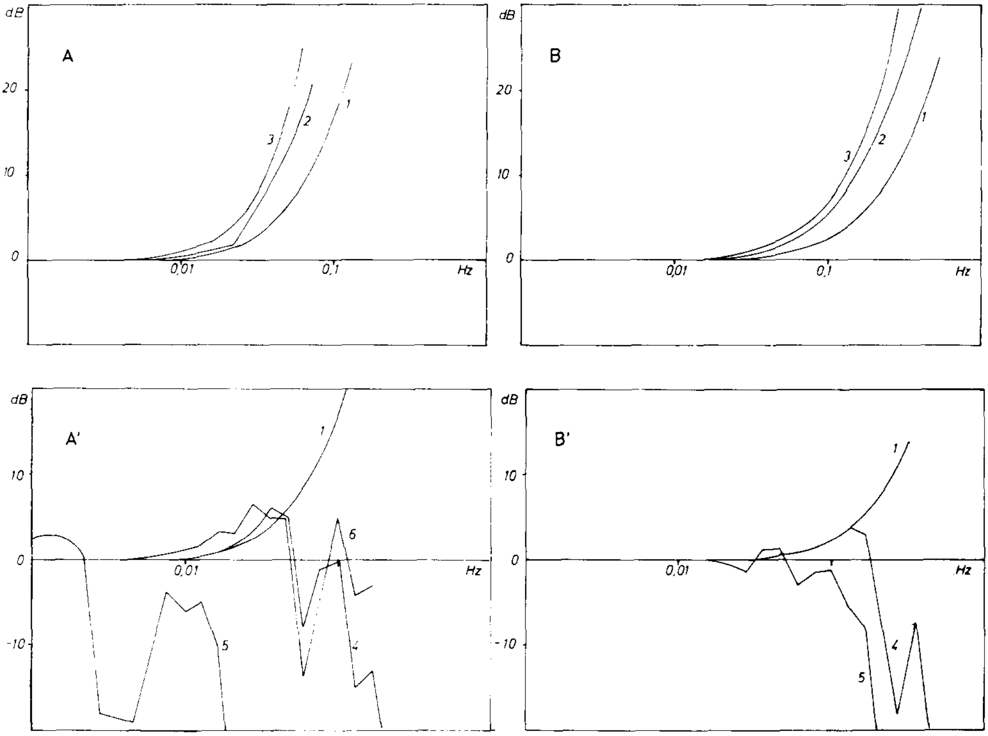

Fig. 4. (A), (A′) Results of Z-transform (ZT) in the model M8. The filter consists of 3 poles and a compensating plant with 3 equal zeros whose values are (1) 1 s, (2) 2 s, (3) 3 s. The signal/noise in the three cases is 140 dB. (4) Same compensating plant as (1) with s/n = 80 dB. (5) Same as (4) with s/n = 60 dB. (6) Same as (3) with s/n = 60 dB. (B), (B′) Results of Z-transform (ZT) in the model M9. The filter consists of 4 poles and 2 zeros and the compensating plant has two equal zeros with values (1) 0.25, (2) 0.5 and (3) 1.0. The signal/noise = 140 dB. (4) Same as (1) with s/n = 100 dB. (5) Same as (1) with s/n = 80 dB.

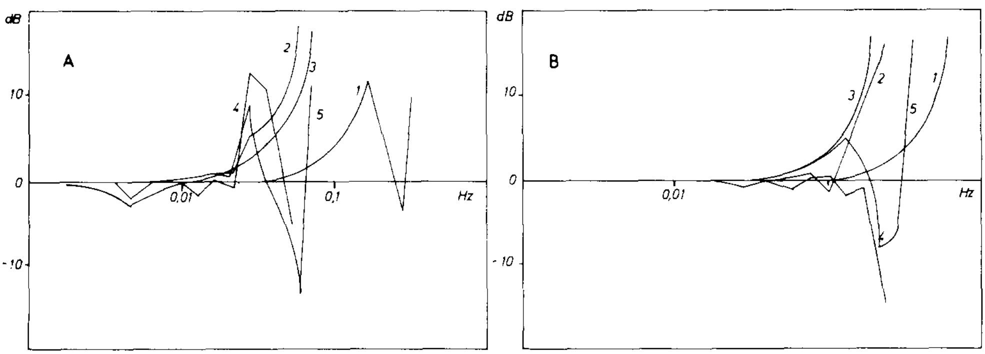

Fig. 5. (A) Harmonic analysis (HA) in the model M8. (1) s/n = 140 dB, $\nu_c = 0.182$ Hz; (2) s/n = 140 dB, $\nu_c = 0.063$ Hz; (3) s/n = 80 dB, $\nu_c = 0.063$ Hz; (4) s/n = 80 dB, $\nu_c = 0.182$ Hz; (5) s/n = 60 dB, $\nu_c = 0.063$ Hz. (B) Harmonic analysis (HA) in the model M9. (1) s/n = 140 dB, $\nu_c = 0.667$ Hz; (2) s/n = 80 dB, $\nu_c = 0.222$ Hz; (3) s/n = 140 dB, $\nu_c = 0.222$ Hz; (4) s/n = 80 dB, $\nu_c = 0.667$ Hz; (5) s/n = 60 dB, $\nu_c = 0.222$ Hz.

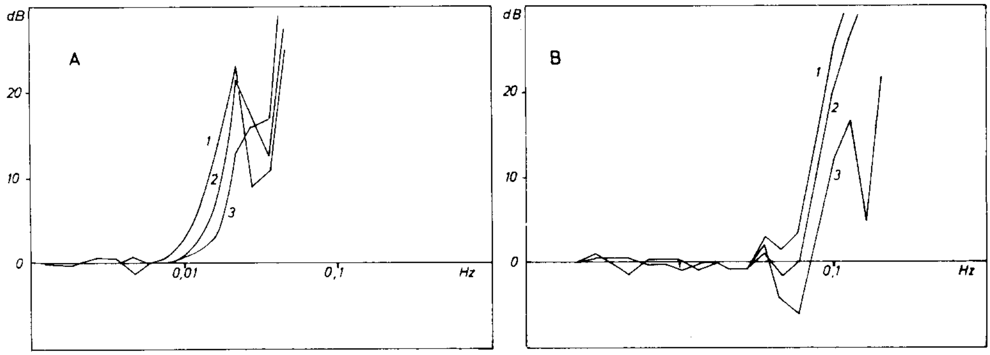

Fig. 6. (A) Optimal control (OC) with the model M8. Signal/noise = 140 dB. (1) $R = 10$ E-05; (2) $R = 6$ E-05; (3) $R = 2$ E-05. (B) Optimal Control (OC) with the model M9. Signal/noise = 140 dB. (1) $R = 15$E-05; (2) $R = 10$E-05; (3) $R = 5$E-05.

thermogenesis. Both the computing time per iteration and the number of iterations rise when a great deal of samples from the thermogram have to be considered. This is the case when the input power in the experiment lasts a long time.

Figure 6 presents the change in the results depending on the number of iterations and the time extent of the thermogenesis.

Optimal control (OC)

In this method the deconvolution problem is rewritten in terms of a tracking problem between the experimental thermogram and a calculated one. The problem is solved in the sense of an optimal control. The main differences with DO are the use of state equations to describe the transfer function of the system, and the non-iterative way in which the optimal control leads to the optimization. The free parameter is now the weight in the performance criterion. The results again strongly depend on the extent of the thermogenesis, and the number of points to be taken into account from the thermogram is limited to the memory occupation of the computer. Figure 7 shows the results obtained with the Optimal Control.

Deconvolution based on the explicit inversion of the heat transport equations in RC models has not been considered. Generally speaking it is difficult to obtain an accurate model of a calorimeter, due to the great number of parameters to be evaluated. On the other hand, the model has to be reduced to very few elements in order to perform the deconvolution. Otherwise the effect of numerical derivatives on the thermogram increases the noise extraordinarily.

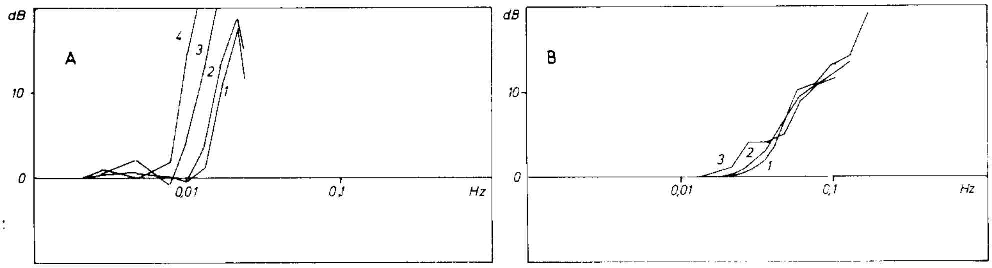

Fig. 7. (A) Dynamic optimization (DO) of M8. Signal/noise = 140 dB. The number of iterations is (1) 60, (2) 45, (3) 30 and (4) 15. (B) Dynamic optimization (DO) of M9. Signal/noise = 140 dB. The number of iterations is (1) 45, (2) 30 and (3) 15.

GENERAL RESULTS

Table 2 shows the memory occupation and computing time for the most significant deconvolutions obtained. To compare their dynamic performances, Fig. 8 presents, in frequency space, the best result for each method together with those obtained by the other methods using equivalent conditions in the calculations.

After the results, and considering that in calorimetric measurements the signal/noise ratio is usually over 50 dB, it seems to be correct to consider IF and ZT as practically equivalent for the purpose of deconvolution. They use only elementary numerical tools and also appear to be the more efficient in time.

Comparatively, the satisfactory results obtained with HA are mainly due to the fact that the whole transfer function is used. This is also the case with DO. On the contrary, OC, IF and ZT use a limited representation of the TF in terms of some poles and zeros. It is also necessary to stress on the point that IF has been presently generalized to deal with time-varying systems [10]. This generalization is also conceptually feasible for ZT and OC [11].

TABLE 2

Memory occupation and computing time for the most significant deconvolutions obtained

Deconvolution method	No. of points handled	Computing time (s) [a]	Memory (kb)
HA	4096	35	~ 60
IF	4000	14	$\lesssim 10$
ZT	4000	14	$\lesssim 10$
OC	1000	27	~ 60
OD [b]	1000	1560	~ 60

[a] In DATA GENERAL Eclipse C-350.

[b] 30 iterations.

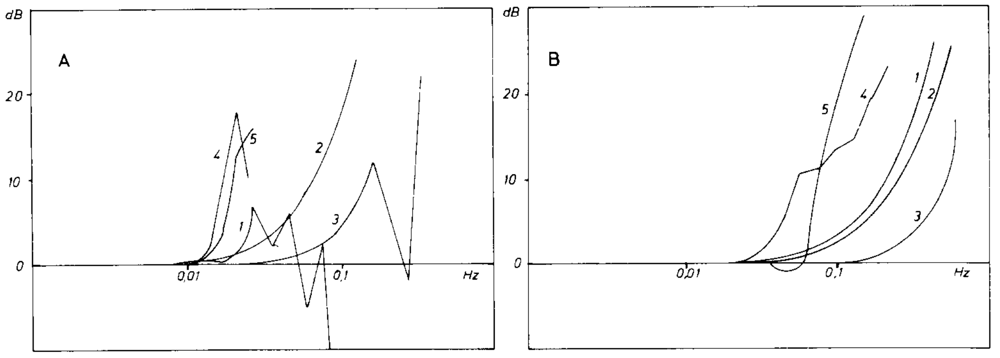

Fig. 8. (A) Comparison of the best results obtained with the different methods for the model M8. (1) IF, (2) ZT, (3) HA, (4) OD, (5) OC. (B) Comparison between the best results obtained for the model M9. (1) IF, (2) ZT, (3) HA, (4) DO, (5) OC.

CONCLUSIONS

(1) IF and ZT appear, after a comparative analysis, as the more efficient in time, more accurate methods of deconvolution in calorimetry.

(2) AH, DO and OC, because they use the whole transfer function, demand a high occupation in memory and a computing time which increases quickly with the number of points considered in the thermogram. The problem may be minimized by sampling with a larger Δt, but this of course means losing kinetic information in the thermogenesis.

(3) IF may nowadays be applied to the thermograms obtained from slightly time-varying calorimetric systems (i.e., in liquid mixtures by continuous injection). ZT and OC should not, conceptually, have any problem in being generalized to time-varying systems, though it has not been brought to practice yet.

REMARK

All times are in seconds. The transfer to relative scale (time $[t/\tau_1]$ or frequency $[\nu\tau_1]$) is easily made ($\tau_1 = 192$ s).

ACKNOWLEDGEMENTS

This work has been developed in the framework of collaboration between the Universities of Palma de Mallorca and Las Palmas de Gran Canaria.

Contacts with different research groups from the Universities of Santiago de Compostela and Barcelona in Spain, Lyon and Marseille in France, and from the Institute of Physical Chemistry in Poland, have been made possible

through different collaboration programs. These contacts have been fundamental in exchanging information on the different deconvolution methods and to evaluate their performances, also, to work with different calorimetric systems.

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