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APPLICATION OF TECHNIQUE SMOOTHING BY CUBIC SPLINE TO INVERSE PROBLEMS OF THERMAL PROCESSES

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Abstract. *This work uses smoothing by cubic spline in order to attenuate noise signal obtained from thermal processes. A signal is generated from an inverse numerical model of the transduction equation considering thermal accumulation and convective heat transfers. As errors in measurement data and ill-conditioning of inverse problem are inevitable, smoothing by cubic spline was implemented as a regularization technique to soften its effects. Numerical tests have shown that the method applied was able to mitigate the ill-conditioning of the numerical model and experimental tests have also evinced the ability of the technique to attenuate noise in real-signal obtained from two thermocouples.*

Keywords: *Inverse problem, regularization, smoothing, cubic spline.*

1. INTRODUCTION

The necessity of different areas of natural sciences or engineering to bond mathematical modeling to experimental data made research on inverse problems to considerably increase in the past decades (Lu, *et al.*, 2010; Park and Lee, 1998). Inverse problems appear in several branches of applied sciences such as engineering, medicine, biotechnology, geophysics, astrophysics, among others (Cezaro and Leitão, 2010).

Inverse problems are related to determining causes by observing effects; the opposite is called direct problem. In other words, direct problems are intended determine the response of a system, given a known input function, and inverse problems consist in determining the input starting from the output function. The inverse problems are known to be ill-posed, that is, at least one of the three conditions (existence, uniqueness and stability) of well-posed problem defined by Hadamard are not met; therefore, the inverse problems are more difficult to solve than the direct problems (Borges and Bazan, 2009; Park and Lee, 1998).

Inverse problems are intrinsically ill-conditioned, meaning the process will be extremely sensitive to experimental and numerical errors, what can seriously jeopardize the obtained results. Due to this instability, the solution of inverse problems is not simple; actually, it gets rather complex, creating the necessity of constant studies in such field. Thus, inverse problems must be treated in order to minimize the introduction of errors that may corrupt results.

According to Tikhonov and Arsenin (1977) inverse ill-posed problems can be associated to well-posed ones, so that the solution of the original problem would be accomplished through associated problem. This theory was called regularization and the best known one was developed by Tikhonov and Arsenin (1977). Since then several regularization methods have been created, each one with a proposed algorithm in order to mitigate the problems caused by function intrinsic ill-conditioning.

In Oliveira, *et al.* (2006) a numerical technique for signal processing was used as a regularization method. The technique employed in Oliveira *et al.* (2006) was the Simplified Method of Least Squares technique or Savitzky-Golay Filters (Savitzky and Golay, 1964), a particular kind of low-pass filter, suitable for smoothing noise. The problem consisted in reconstructing, in real time, the temperature of the original process from a distorted, delayed and noisy signal, measured by an intrusive gauge. The problem formulation took into account thermal accumulation, convection and radiation. Numerical and experimental results have shown that the technique proposed in Oliveira *et al.* (2006) allow reconstruction of process temperature under real experimental conditions with relatively high levels of noise. However, the probe time constant and the radiation coefficient depend on convection coefficient, previously determined by a minimization process, what is not appropriate for real-time processing, since the temperature reconstruction process depends on outdated information.

However, the optimal smoothing depends on the assortment of appropriate algorithm and optimal smoothing parameters that will reach the best commitment between noise reduction and signal recovery. Several methods, such as moving average filtering, simplified least squares method, splines, Fourier and wavelet transforms have been used in the treatment of noise. The main purpose of applying such methods is the improvement of signal-to-noise ratio (Jakubowska, 2011).

Among the several regularization methods, the spline function has wide application in data interpolation, because spline function is a curve constructed of polynomial segments which are subject to conditions or continuity of their points. But if data are originated from experiments, smoothing by splines has been more used, especially after the first algorithm was provided by Reinsch (1967).

This work aims to ease noise signal obtained from thermal processes through smoothing by cubic splines. Cubic spline smoothing was chosen because it ensures overall data smoothing; this method tends to be more stable and to cause less possibility of data variation. A signal is generated from an inverse discrete numerical model of the transduction equation considering thermal accumulation and convective heat transfer. Numerical tests show that the technique applied was able to mitigate the ill-conditioning of the inverse numerical model, and experimental tests also show the capability of the technique to attenuate noise in actual signal obtained from two thermocouples.

2. METHODOLOGY

2.1 Mathematical formulation of the inverse problem

Figure 1 represents graphic scheme of the inverse problem studied in this work. Two thermocouples are inserted into a reagent emulsion; first thermocouple provides the actual temperature of the process, T_{proc} and second thermocouple is sheathed and provides the temperature of flow (indicated), T_{ind}.

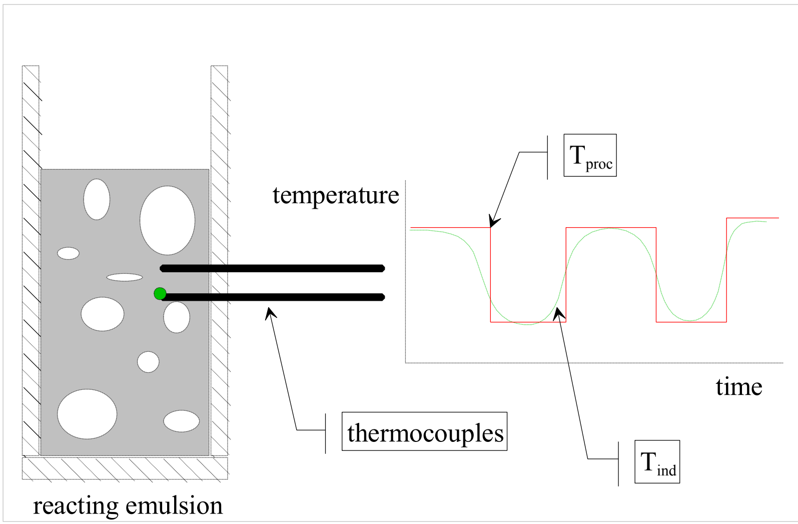

Figure 1. Graphic scheme of inverse problem

Temperatures T_{proc} and T_{ind} are differentiated by the distortions caused by the thermal accumulation of the sheathing of thermocouple and by the delays due to the physical mechanisms that underlie the modes of heat transfer, such as convection and radiation.

In this work, it was considered thermal accumulation and convective heat transfers to the mathematical formulation of the inverse heat transfer problem, so the equation becomes:

$$MC\frac{dT_{ind}}{dt} - hA\left(T_{proc} - T_{ind}\right) = 0 \tag{1}$$

where M (kg) is sheath mass and C (J/kgK) is the specific heat of the thermal accumulation, A (m^2) is the area and h (W/m^2K) is the convection coefficient of heat transfer. Heat transfer by conduction through the cable of the thermocouples was disregarded, since the area of the wire is considered minimal. Dividing Eq. (1) by hA, it is obtained:

$$\tau\frac{dT_{ind}}{dt} - \left(T_{proc} - T_{ind}\right) = 0 \tag{2}$$

where $\tau = \dfrac{MC}{hA}$ is the time constant of the probe, that is, the temperature increase caused by heat accumulation over heat transferred by convection.

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Equation (2) can be discretized in time by delayed finite differences method with indices i and $i-1$ indicating that the variable refers in times $t_i = i\Delta t$ and $t_{i-1} = (i-1)\Delta t$, and Δt step in time. Thus Eq. (2) can be rewritten as:

$$\frac{\tau_i}{\Delta t}\left(T_{ind,i} - T_{ind,i-1}\right) - \left(T_{proc,i} - T_{ind,i}\right) = 0 \tag{3}$$

Thus, the direct and inverse problems are expressed, respectively, Eq. (4) and Eq. (5), calculating the output (T_{ind}) of the known input (T_{proc}), Eq. (4), and calculating the input (T_{proc}) of the known output (T_{ind}), Eq. (5), respectively as:

$$T_{ind,i} = \frac{1}{\frac{\tau}{\Delta t} + 1}\left(T_{proc,i} + \frac{\tau}{\Delta t} T_{ind,i-1}\right) \tag{4}$$

$$T_{proc,i} = T_{rec,i} = \frac{\tau}{\Delta t}\left(T_{ind,i} - T_{ind,i-1}\right) + T_{ind,i} \tag{5}$$

Due to the intrinsic nature of the ill-conditioning of inverse problems, their solutions may be corrupted by noise in input data, what justifies the study of smoothing methods for treating the results. As a matter of notation, the temperature obtained from the inverse problem Eq. (5) will be named reconstructed temperature (T_{rec}), so it will not be mistaken as the actual process temperature (T_{proc}).

2.2 Method of smoothing by cubic spline

The smoothing by cubic spline brings in its formulation the construction of a new function, through spline function and regularized points that will be determined in order to minimize the error between the distances of the given points and the smoothed ones. The method requires the determination of parameters, which, though flexible, had its characteristics investigated in this work, because they control the strength of the smoothing and delay of regularized signal over the reconstructed signal.

The method of smoothing by cubic splines described in this article was based on the works of Reinsch (1967), Pollock (1993) and Weinert (2009). The temperature is restored in time t_i given by:

$$T_{rec,i} = T_{reg,i} + \varepsilon_i \tag{6}$$

where ε is the error between the original points T_{rec} from the inverse problem Eq. (5) and the smoothed ones T_{reg} obtained after the application of the regularization method. In this case, the reconstitution of T_{reg} will be through the construction of a function $S(t)$ that minimizes:

$$L = \lambda \sum_{i=1}^{n} \left(\frac{T_{rec,i} - T_{reg,i}}{T_{rec,i}}\right)^2 + (1-\lambda)\int_{t_0}^{t_n} \left(S''(t)\right)^2 dt \tag{7}$$

where λ is the parameter that controls the smoothing degree and n the total amount of points. The second term of Eq. (7) can be rewritten as a sum of the second derivatives of each of the intervals, as:

$$\int_{t_0}^{t_n} \left(S''(t)\right)^2 dt = \sum_{i=0}^{n-1} \int_{t_i}^{t_{i+1}} \left(S''(t)\right)^2 dt \tag{8}$$

Each spline is composed of cubic segment, then the second derivative at any interval is a linear function, with the independent term $2b_i$ in t_i, $2b_{i+1}$ in t_{i+1} and $H_i = t_{i+1} - t_i$, then Eq. (8) becomes:

$$\int_{t_0}^{t_n} \left(S''(t)\right)^2 dt = 4\int_0^{h_i} \left(b_i \left(1 - \frac{t}{H_i} \right) + b_{i+1} \frac{t}{H_i} \right)^2 dt \tag{9}$$

Solving the Eq. (9) there is as follows:

$$4\int_0^{h_i} \left(b_i \left(1 - \frac{t}{H_i} \right) + b_{i+1} \frac{t}{H_i} \right)^2 dt = \frac{4H_i}{3}\left(b_i^2 + b_i b_{i+1} + b_{i+1}^2\right) \tag{10}$$

It is possible to rewrite the function $S(t)$ and $S''(t)$ as to depend on variables b_i and $T_{reg,i}$. Considering the coordinates $(t_i, T_{reg,i})$, $(t_{i+1}, T_{reg,i+1})$ and the implicit conditions:

$$S_i(t_i) = T_{reg,i} \tag{11}$$

$$S_i(t_{i+1}) = T_{reg,i+1} \tag{12}$$

$$S_i''(t_i) = 2b_i \tag{13}$$

$$S_i''(t_{i+1}) = 2b_{i+1} \tag{14}$$

Equation (11) and Eq. (12) are respectively, an identity and equality. Equation (12) can be opened as a cubic function as follows:

$$a_i H_i^3 + b_i H_i^2 + c_i H_i + T_{reg,i} = T_{reg,i+1} \tag{15}$$

Isolating c_i from Eq. (15), it is obtained:

$$c_i = \frac{T_{reg,i+1} - T_{reg,i}}{H_i} - a_i H_i^2 + b_i H_i \tag{16}$$

Equation (13) and Eq. (14) are an identity and equality, respectively. Equation (14) can be opened as the second derivative of Eq. (15) as:

$$2b_{i+1} = 6a_i H_i + 2b_i \tag{17}$$

Isolating a_i from Eq. (17) it is obtained:

$$a_i = \frac{b_{i+1} - b_i}{3H_i} \tag{18}$$

Substituting Eq. (18) in Eq. (16):

$$c_i = \frac{T_{reg,i+1} - T_{reg,i}}{H_i} - \frac{1}{3}\left(b_{i+1} - 2b_i\right)H_i \tag{19}$$

Deriving Eq. (15) and isolating c_i gives:

$$3a_{i-1}H_{i-1}^2 + 2b_{i-1}H_{i-1} + c_{i-1} = c_i \tag{20}$$

Equalizing Eq. (19) and Eq. (20) and rearranging it:

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$$b_{i-1}H_{i-1}+2b_i\left(H_{i-1}+H_i\right)+b_{i-1}H_i=\frac{3}{H_i}\left(T_{reg,i+1}-T_{reg,i}\right)-\frac{3}{H_{i-1}}\left(T_{reg,i}-T_{reg,i-1}\right) \tag{21}$$

According to the condition of the natural spline, the first and the last element of vector $\{b\}$ are zero, that is, $b_0=b_n=0$, with $i=1,2,\cdots,n-1$. Equation (21) can be rewritten as a matrix system:

$$\underbrace{\begin{bmatrix} p_2 & H_2 & 0 & \cdots & 0 & 0 \\ H_2 & p_3 & H_3 & \cdots & 0 & 0 \\ 0 & H_3 & p_4 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & p_{n-2} & H_{n-2} \\ 0 & 0 & 0 & \cdots & H_{n-2} & p_{n-1} \end{bmatrix}}_{[a]}\underbrace{\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{n-2} \\ b_{n-1} \end{bmatrix}}_{\{b\}}=\underbrace{\begin{bmatrix} r_1 & f_2 & r_2 & 0 & \cdots & 0 & 0 \\ 0 & r_2 & f_3 & r_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & r_{n-2} & 0 \\ 0 & 0 & 0 & 0 & \cdots & f_{n-1} & r_{n-1} \end{bmatrix}}_{[F]}\underbrace{\begin{bmatrix} T_{reg,1} \\ T_{reg,2} \\ \vdots \\ T_{reg,n-1} \\ T_{reg,n} \end{bmatrix}}_{\{T_{reg}\}} \tag{22}$$

where,

$$H_i=t_{i+1}-t_i \tag{23}$$

$$p_i=2\left(H_{i-1}+H_i\right) \tag{24}$$

$$r_i=\frac{3}{H_i} \tag{25}$$

$$f_i=-\left(\frac{3}{H_{i-1}}+\frac{3}{H_i}\right)=-\left(r_{i-1}+r_i\right) \tag{26}$$

Rewriting Eq. (22) in matrix notation:

$$[a]\{b\}=[F]\{T_{reg}\} \tag{27}$$

This notation can be used in Eq. (10) and substituted in Eq. (7), thus:

$$L=\lambda\{T_{rec}\}^{-1}\left(\{T_{rec}\}-\{T_{reg}\}\right)^2+\frac{2}{3}(1-\lambda)[a]\{b\}^2 \tag{28}$$

By isolating $\{b\}$ the Eq. (27), as:

$$\{b\}=[a]^{-1}[F]\{T_{reg}\} \tag{29}$$

Equation (29) there are two unknown variables, $\{b\}$ and $\{T_{reg}\}$, then one of them should be replaced by another known variable for the system to be solved. Substituting Eq. (29) in Eq. (28), the terms of Eq. (30) now depend on T_{reg}:

$$L\left(\{T_{reg}\}\right)=\lambda\{T_{rec}\}^{-1}\left(\{T_{rec}\}-\{T_{reg}\}\right)^2+\frac{2}{3}(1-\lambda)[a]^{-1}[F]^2\{T_{reg}\}^2 \tag{30}$$

To optimize the values of $\{T_{reg}\}$, Eq. (30) is minimized by differentiation with the respective $\{T_{reg}\}$ and result is equaled to zero, thus:

$$-2\lambda\{T_{rec}\}^{-1}\left(\{T_{rec}\}-\{T_{reg}\}\right)+\frac{4}{3}(1-\lambda)[a]^{-1}[F]^2\{T_{reg}\}=0 \tag{31}$$

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Rearranging Eq. (31) and substituting in Eq. (29):

$$\lambda\{T_{rec}\}^{-1}\left(\{T_{rec}\}-\{T_{reg}\}\right)=\frac{2}{3}(1-\lambda)[F]\{b\} \tag{32}$$

Multiplying Eq. (32) by $\lambda^{-1}[F]\{T_{rec}\}$ and rearranging it using identity Eq. (27) it is obtained:

$$\underbrace{\left([a]+\mu[F]^2\right)}_{[E]}\{b\}=\underbrace{[F]\{T_{rec}\}}_{[D]} \tag{33}$$

where,

$$\mu=\frac{2(1-\lambda)}{3\lambda} \tag{34}$$

Rewriting Eq. (33) and isolating the vector $\{b\}$ as:

$$\{b\}=[E]^{-1}[D] \tag{35}$$

Once found the vector $\{b\}$, the smoothing vector $\{T_{reg}\}$ can finally be written:

$$\{T_{reg}\}=\{T_{rec}\}-\mu\{b\}[F] \tag{36}$$

Data $\{T_{rec}\}$ will be smoothed according to the following steps:

1. Assemble the matrices $[a]$ and $[F]$ of the Eq. (22) with the values described in Eq. (23), Eq. (24), Eq. (25) and Eq. (26).
2. Build the matrices $[E]$ and $[D]$ as Eq. (33).
3. Determine the vector $\{b\}$ from the Eq. (35).
4. Calculate the smoothing vector $\{T_{reg}\}$ with the smoothing modified parameter μ chosen previously.

3. RESULTS

The described algorithm was implemented in the software MATLAB®, which has a toolbox for smoothing by cubic spline; however there is not flexibility in all the parameters this job requires, for this reason a new implementation was carried out according to the project needs.

Numerical tests were performed in order to evaluate and analyze the implemented smoothing method by cubic spline and its parameters. It was generated a signal which simulates T_{proc}, with maximum temperature of 373 K and minimum of 363 K, according to a square nature wave. T_{ind} is obtained through the direct problem, Eq. (4), which is inserted with random noises and T_{rec} is obtained through inverse problem, Eq. (5). To soften T_{rec} which intrinsic nature of ill-conditioning amplified noises during the inverse process, it was applied a smoothing signal algorithm through cubic spline method.

The input data for the numerical experiment are: $M=4{,}7\times10^{-6}$ kg, $C=3{,}8\times10^{-2}$ J /kgK, $A=3{,}14\times10^{-6}$ m^2, $h=5{,}5\times10^{2}$ W /m^{2}K, resulting in a time constant $\tau=1{,}0342$ s, $\Delta t=0{,}001$ s and $\text{noise}=0{,}01$ K.

Figure 2 shows the signals of T_{proc}, of the direct problem T_{ind} and of inverse T_{rec} and T_{reg} that is the signal of the regularized temperature. Thus, it is observed that the smoothing by cubic spline was able to smoothen T_{rec} and therefore reconstruct T_{proc}.

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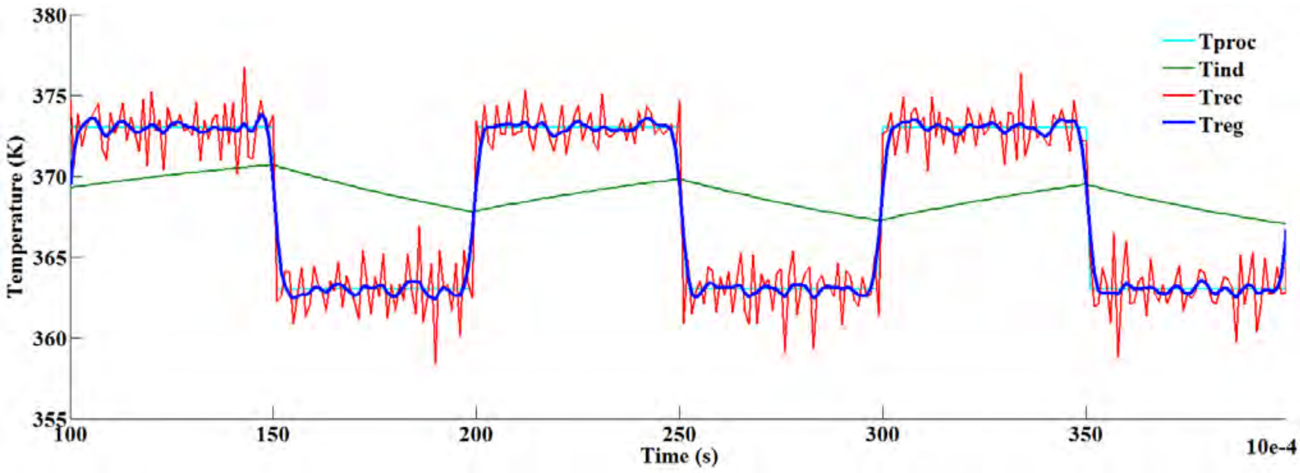

Figure 2. Signal of temperature smoothed by cubic spline

In order to get the best performance of the algorithm and thus the minimum error between T_{proc} and T_{reg}, some parameters must be determined a priori, as λ and $3/H$. Parameter λ, Eq. (34), regulates the degree of smoothness that goes from linear regression to interpolation and in Eq. (21) it is possible to add weights to the term $3/H$, and this way control the strength of the smoothing; term $3/H$ refers weight one. Table 1 shows variation of parameter λ by the weight placed along with $3/H$, with respective errors calculated according to Eq. (37):

$$E = \sqrt{\frac{\sum_{i=1}^{n}\left(T_{proci} - T_{regi}\right)^2}{n}} \tag{37}$$

Table 1. Average of errors between the T_{proc} and the T_{reg}, in accordance with the variation of λ and the weight

$H \setminus \lambda$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
H	194.555	39.525	17.66	9.48	8.725	9.895	11.345	13.935	14.775	15.845
$1/H$	195.435	40.005	17.16	8.73	7.9	10.36	12.67	13.7	14.72	16.785
$2/H$	97.94	31.995	13.215	6.26	7.415	10.37	11.945	13.685	15.42	15.82
$3/H$	69.37	25.46	10.14	4.98	7.555	10.28	11.78	12.5	14.505	15.225
$4/H$	71.615	30.97	11.565	5.125	8.025	9.945	13.09	14.02	15.07	16.96
$5/H$	78.88	24.505	12.795	5.22	8.105	10.355	12.07	13.66	14.67	16.09
$6/H$	81.465	28.605	13.27	5.46	7.95	10.96	11.665	13.535	14.86	17.435
$7/H$	77.32	29.365	12.88	5.46	7.62	10.845	12.16	14.12	15.91	17.57
$8/H$	85.36	33.62	13.155	5.74	8.43	10.575	12.48	15.405	16.215	16.96
$9/H$	85.96	33.985	13.785	5.95	7.8	10.595	11.815	14.29	14.905	16.195
$10/H$	86.07	32.125	14.66	5.98	8.69	10.705	12.135	14.795	13.78	16.12

According to Tab. 1 it may be determine the best weight for H and the best λ as being respectively $3/H$, this is, weight 1 and $\lambda = 0{,}4$, as shows Fig. 2, since there is no delay in regularized signal and minimum error.

The parameter λ between 0,1 and 0,3 is not indicated, since in accordance with the obtained results they are accompanied by a delay in relation to T_{rec}. For λ between 0,4 and 0,6 is the best range of smoothing, therefore, does not show delay, and errors are low. For λ between 0,7 and 0,9 they are closer to interpolation than smoothing, although not accompanied by delay. While $\lambda = 1{,}0$ represents an interpolation of data, since the vector smoothing has the same points.

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In respect to the weights, values between $1/H$ to $6/H$ or even just H smooth moderately depending on λ, and values between $7/H$ and $10/H$ show a strong smoothing as shown in Fig. 3, which smoothing is performed for $10/H$ and $\lambda = 0{,}4$, this is, $3{,}3 \times 3/H$.

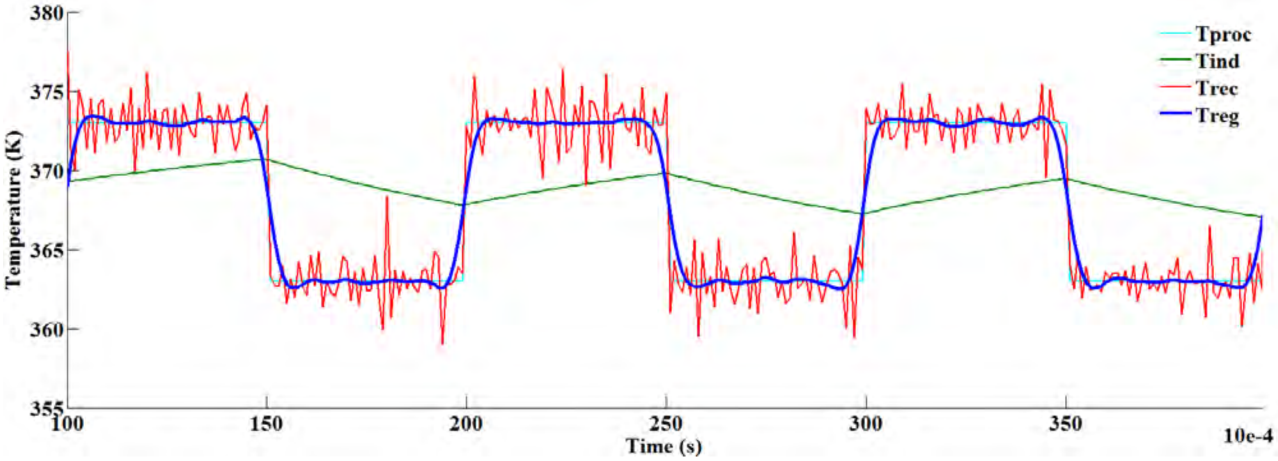

Figure 3. Strong smoothing with parameters $10/H$ and $\lambda = 0{,}4$

The studied parameters must be adapted according to the interference of the level of noise associated to the signal. Fig. 4a and Fig. 4b show the errors related to low and high noises, respectively, among the three best weights H and the three best λ as Tab. 1. For example, for a noise of 0,001 K, in accordance with Fig. 4a the best λ and H are $\lambda = 0{,}6$ and $3/H$, Fig. 5, to a noise of 0,05 K in accordance with the Fig. 4b the best λ and H are $\lambda = 0{,}4$ and $5/H$, Fig. 6.

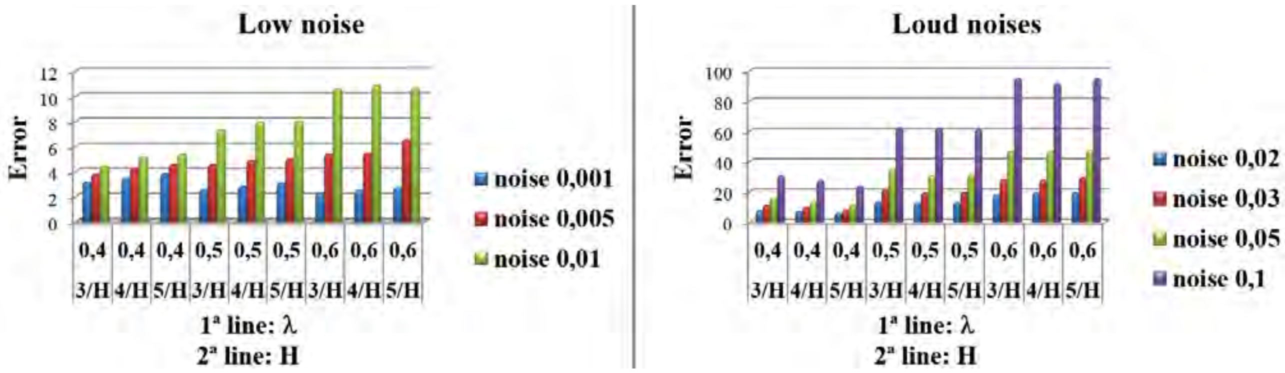

Figure 4. Errors in respect to noises and the best λ and H. (a) Low noise between 0,001 and 0,01, (b) Loud noises between 0,02 and 0,1

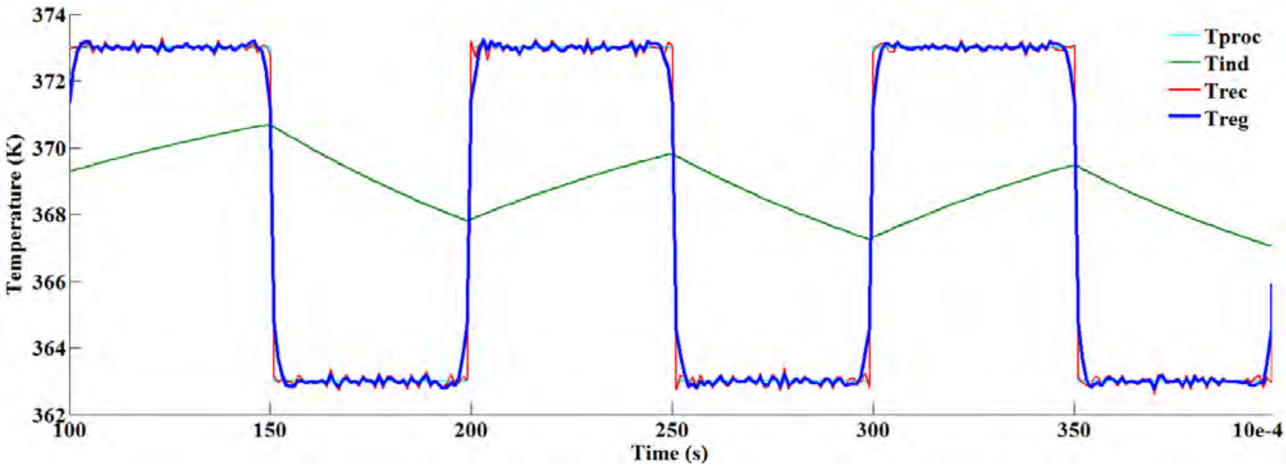

Figure 5. Signal smoothing for $noise = 0{,}001$ K, $\lambda = 0{,}6$ and $3/H$

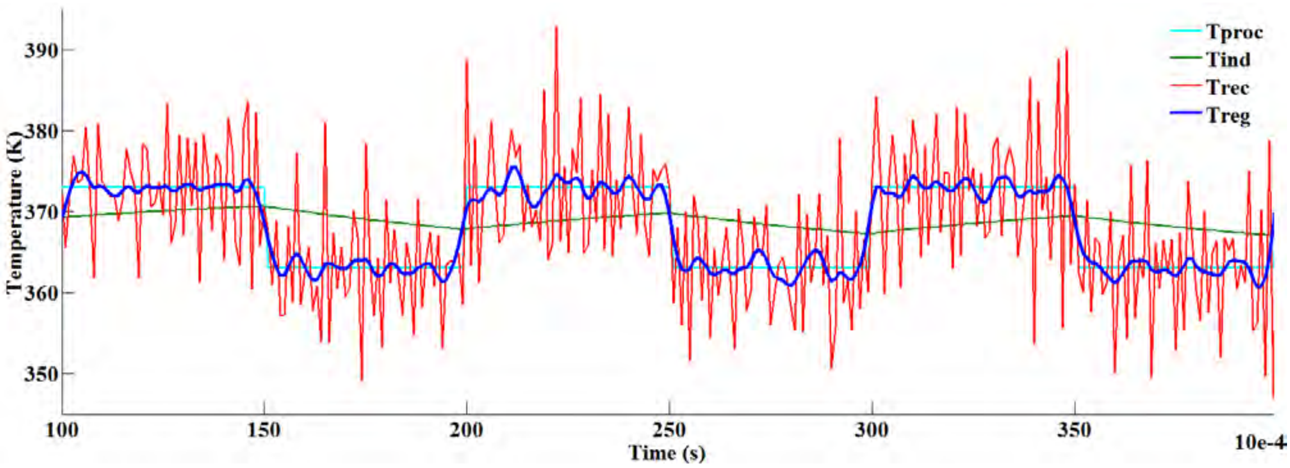

Figure 6. Signal smoothing under $noise = 0{,}05$ K, $\lambda = 0{,}4$ and $5/H$

For validating the efficiency of the algorithm, experimental tests were conducted with temperature signals assigned by author Juliana de Oliveira, acquired during her doctorate performed from 2002 to 2006, at Thermal and Fluid Engineering Laboratory, School of Engineering of São Carlos, University of São Paulo, (NETeF - EESC - USP - São Carlos), which input data are: $\tau = 1{,}3\,\text{s}$ (Oliveira, 2006). It is observed in Fig. 7 that the smoothing by cubic spline was cable to reconstruct T_{proc}; however peaks appeared in T_{reg} that are considered a combination between the method of smoothing by cubic spline and the fact that the convective thermal processes are dependent on the convective coefficient, which in this work are previously estimated.

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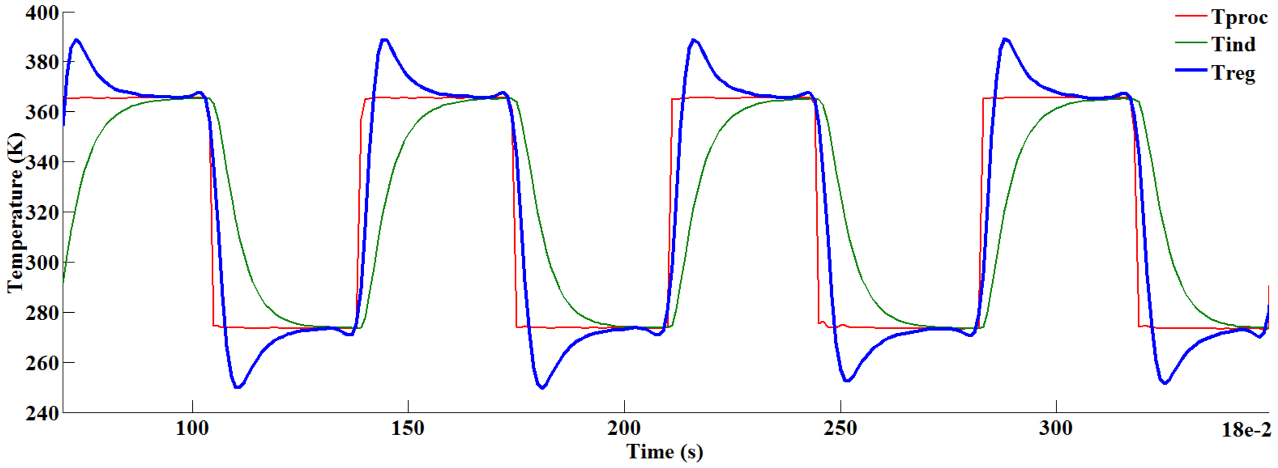

Figure 7. Reconstruction of the temperature signal obtained from experimental tests

4. CONCLUSION

This paper proposed the reconstruction of temperature of thermal processes that, due to ill-conditioning of inverse problem noise amplification occurs and therefore, requires a method of regularization which, in this case, was the smoothing by cubic splines. The smoothing by cubic spline is an off-line method of regulation, that is, it is necessary the set of points that will be smoothed to be complete so that the process may be started. Numerical and experimental tests showed its efficiency, combined with analysis of flexible parameters that have been set to optimize the results of this project, in addition to offering more technical stability. Resulting from analysis of numerical and experimental tests, the proceeding of this work will be focused on the addition of radiation in equating the problem, and at the same time, another work will be carried in order to determine the best convection coefficient, which thermal processes are dependent of.

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6. RESPONSIBILITY NOTICE

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