Effect of Smoothing Methods on the Results of Different Inverse Modeling Techniques

I. Felde [1], T. Réti [2], G. Sánchez Sarmiento [3], M.G. Palandella [3] , G.E. Totten [4], and X.L. Chen [5]

1) Bay Zoltán Institute for Materials Science and Technology, Budapest, Hungary.
2) Bánki Donát Polytechnic, Budapest, Hungary.
3) Universidad de Buenos Aires, Facultad de Ingeniería. Buenos Aires, Argentina.
4) Dow Chemical, Tarrytown, NY, USA.
5) Oregon Graduate Institute of Science and Technology, Portland, USA.

ABSTRACT

The quantitative evaluation of quenchants cooling power is indispensable for the computer simulation of steel hardening processes. The heat transfer coefficient (HTC) or heat flux is used as boundary condition to simulate the cooling process during quenching. The HTC can be estimated by Inverse Heat Conduction Problem (IHCP) software using the most important input data, the measured cooling curves. The calculated heat transfer coefficient substantially depends on the noisiness of the measured cooling curves. In this paper the performance of different data filtering techniques has been studied. Comparative analysis of smoothing methods has been demonstrated by using HTC calculations that are based on the cooling curves filtered by various techniques. Suggestions have been made for better filtering and smoothing of noisy data.

Introduction

The cooling power of a quenchant is generally characterized by the heat transfer coefficient (HTC) between the metal surface and the quenchant, that strongly depends on the surface temperature of the piece. HTC is used as boundary condition to simulate the heat treating process of steels by computational techniques, solving the heat conduction equation coupled with phase transformation of the material [(1)] .

Typically, HTC are derived from experimental temperature – time data measured by thermocouples (cooling curves) placed within some standardized probes [(2)], and solving the heat conduction problem coupled with the microstructural changes. The mathematical procedure of obtaining HTC as a function of temperature, from cooling curves for a given material and geometry, is an ill-posed numerical problem of great complexity [(3)]. The numerical difficulties of this problem are strongly increased by statistical errors in the measured cooling curves ("noise"), which mainly affect the resulting HTC. By this reason, application of noise filtering techniques to measured cooling curves after the data acquisition process is of great importance for that purpose.

Several smoothing algorithms are available in the literature. Between them, the moving-average technique and the algorithm of Savitzky – Golay [(4)] are well known and are frequently used for this purpose. Recently, a computational method based on the classical Fourier analysis for filtering end encoding of measured or computed quench data, has been presented by Felde et al [(5)]. This numerical technique was designed primarily to generate smoothed cooling curves, temperature rate curves and HTC functions. The performance and the accuracy of the method was demonstrated in ref. 5, on examples with superimposed noise that was produced by a random number generator.

An application of this smoothing technique to real cooling curve analysis is now described in this paper, obtaining temperature dependent HTC of the different quenchants by means of the INC-PHATRAN Code [(6-8)]. The results without smoothing were previously presented in ref. 9. Cooling curves measured by thermocouples at the center of Stainless Steel 304 cylindrical probes of 1" diameter and 2" long, quenched in helium gas and also in oil, was used for the comparative analysis. The Fourier technique with several different quantity of coefficients, and also the Savitzky – Golay method, has been applied to the original cooling curves. Good enhancements of the HTC resulting from these curves are demonstrated at follows.

Brief description of the filtering technique.

The formal mathematical background of the method was described in ref. 5 and is briefly summarized here. It is based on the following considerations: Let us assume that the finite set of the so-called noisy data which are obtained by measurement or computation is represented by data pairs of real numbers (t_i, y_i) for i = 0,1,2,…,2N, where 2N stands by the number of data pairs. In practice, value of N ranges from 100 to 10000. Data pairs (t_i, y_i) are considered as samples values of a continuous "noisy" function $Y_A = Y_A(t)$ which is defined in the interval [t_s, t_f], and for which $y_i = Y_A(t_i)$ is fulfilled for any $t_i = t_0 + i\,(t_f - t_s)/2N$, where i = 0, 1, 2,…, $2N$, and $t_0 = t_s$, $y_0 = y_s$ and $t_{2N} = t_f$, $y_{2N} = y_f$ are fulfilled, respectively (See Fig.1).

In order to eliminate or reduce the noise and to obtain smoothed data pairs, digital filters of various type can be applied. As it is known, a digital filters is designated to remove those components of the signal, called noise, which are unrelated to the measured or computed magnitude [4].

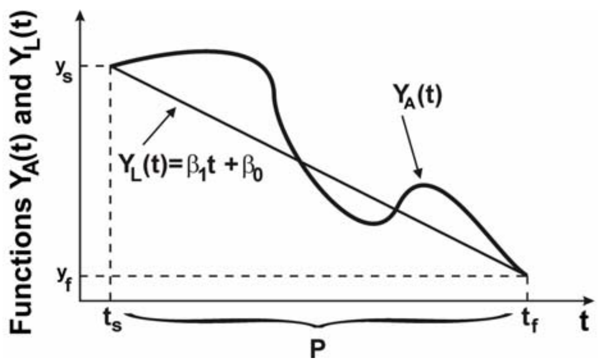

Figure 1. Principle of the computational method based on Fourier analysis

In order to apply the Fourier analysis to filtering purposes, a periodical function $Y_P(t)$ should be constructed from $Y_A(t)$ as follows:

$$Y_P(t) = Y_A(t) - Y_L(t) \qquad (1)$$

where:

$$Y_L(t) = \beta_1 t + \beta_0 \qquad (2)$$

$$\beta_1 = \frac{y_f - y_s}{t_f - t_s} = \frac{y_{2N} - y_0}{t_{2N} - t_0} \qquad (3)$$

$$\beta_0 = y_s - \beta_1 t_s = y_0 - \beta_1 t_0 \qquad (4)$$

In ref. 5 is demonstrated that Y_A (t) may be approximated by a truncated Fourier series:

$$Y_{F,M}(t) = Y_M(t) + Y_L(t) = \beta_0 + \beta_1 t + \frac{a_0}{2} + \sum_{k=1}^{M} a_k \cos\left(k\frac{2\pi}{P}t\right) + b_k sin\left(k\frac{2\pi}{P}t\right) \qquad (5)$$

where:

$$a_k = \frac{1}{N}\sum_{k=1}^{2N-1} Y_i \cos\left(i\frac{k\pi}{N}\right) \qquad (6)$$

$$b_k = \frac{1}{N}\sum_{k=1}^{2N-1} Y_i sin\left(i\frac{k\pi}{N}\right) \qquad (7)$$

$$Y_i = y_i - (\beta_1 t_i + \beta_0) \qquad (8)$$

for i = 0, 1, 2,…$2N$ and k = 0, 1, 2,…, M,

and $t_s \le t \le t_f$.

In Equation (5) integer M is the maximum number of Fourier coefficient pairs used for approximation. Function $Y_{F,M}(t)$ can be used directly for calculating the "smoothed value" of y_i for any t_i on the whole interval $t_s \le t_i \le t_f$.

It is important to note that the value of M should be selected carefully, as a result of compromises. It is obvious, that if M is decreased, this implies that the accuracy of approximation will decrease simultaneously, on the other hand, increasing of M leads to the decrease in the efficiency of noise reduction. It the following it will be shown that the optimum value of M, which ensure the fulfillment of both requirements, ranges from 8 to 16.

The INC-PHATRAN Code

INC-PHATRAN (INverse Conduction coupled with PHAse TRANsformation) [6-8] is a program that may be applied to simulate a great variety of heat treatment processes, in planar geometry as well as in axysimmetrical ones, by means of a finite element approach. The corresponding heat transfer coefficients can be calculated with its help, if cooling curves taken from different locations of the heat treated component are provided. The model is based on a numerical optimization algorithm which includes a module responsible for the calculation on time and space the temperature distribution and its coupled microstructure evolution. The transformation from austenite to ferrite, perlite and martensite is governed by the appropriate TTT curve and also by the Avrami's approximation. The temperature variation, as measured by means of thermocouples at different positions in the component, are used as input for the program. The program calculates the time variation of the heat transfer coefficients, together with the temperature and distribution of phases, and their variation in time throughout the component.

Experimental procedure

Stainless Steel 304 cylindrical probes of 1” diameter and 2” long (see figure 1) were used to measure the cooling curves. They were quenched in helium gas with 5 different concentrations and a temperature of 28 ºC, and also in oil at 28, 30, 33 and 36 ºC. Thermocouples were inserted in the center of each sample. A specially prepared testing apparatus was used to control the temperature.

The thermocouples were connected to a computer to carry out the data acquisition process, with a known frequency. These curves were then kept in numerical files which were afterwards used to feed INC-PHATRAN. Figures 2 and 3 show the measured cooling curves for both quenchants respectively. Model INC-PHATRAN were used to calculate the temperature dependent heat transfer coefficient corresponding to the 8 cooling curves showed in figures 2 and 3. Values of the thermal conductivity and the specific heat as depending of temperature, and of the density, are indicated in table 1.

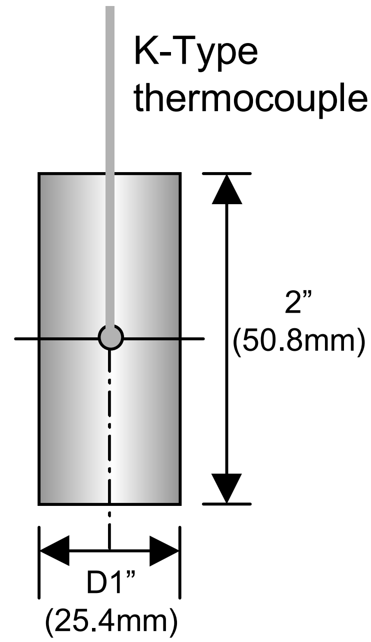

Figure 1. Schematic of 1” diameter 2” long stainless steel probe.

Temperature dependent thermal conductivity		Temperature dependent Specific Heat		Density
Temperature [ºC]	Conductivity [w/m^{2}K]	Temperature [ºC]	Specific heat [J/kg.K]	[kg/m^3]
100.	16.3	38.	527.	7650.
204.	17.1	93.	549.	
427.	21.1	204.	567.	
500.	21.5	316.	586.	
649.	24.7	371.	601.	

Table 1: Thermophysical constant of the material considered in the modeling.

		1” diameter probes quenched in Helium					1” diameter probes quenched in oil			
		2.5x, 28 °C	3.0x, 28 °C	3.5x, 28 °C	4.0x, 28 °C	4.5x, 28 °C	Oil, Ag 28	Oil, Ag 30	Oil, Ag 33	Oil, Ag 36
Original		6.90	0.18	1.73	0.75	1.14	2.31	2.22	0.75	0.32
Savitzky-Golay	n_R=5	8.28	0.19	1.90	1.19	1.34	1.96	1.87	0.91	0.36
	n_R=11	7.00	0.18	1.82	0.93	1.06	2.09	1.32	0.94	0.35
	n_R=15	6.69	0.16	1.96	0.93	0.95	1.41	1.23	0.89	0.27
	n_R=17	6.41	0.22							
	n_R=21	8.71	0.24	1.84	0.74	1.33	0.41	1.24	1.14	0.26
	n_R=25	5.84	1.84	2.63	0.85	1.34	0.21	0.93	0.74	0.20
Fourier	M=20	6.25	1.83	2.23	0.94	1.16	1.08	3.08	2.49	1.30
	M=30	13.91	1.09	1.72	0.64	0.97	1.95	1.80	2.57	0.76
	M=40	6.15	1.88	2.56	0.58	1.02	1.46	2.31	2.58	0.60
	M=50	11.33	1.83	2.23	0.94	1.16	1.08	3.08	2.49	1.30

Table 2: Mean quadratic difference between measured (and then smoothed) and calculated temperatures.

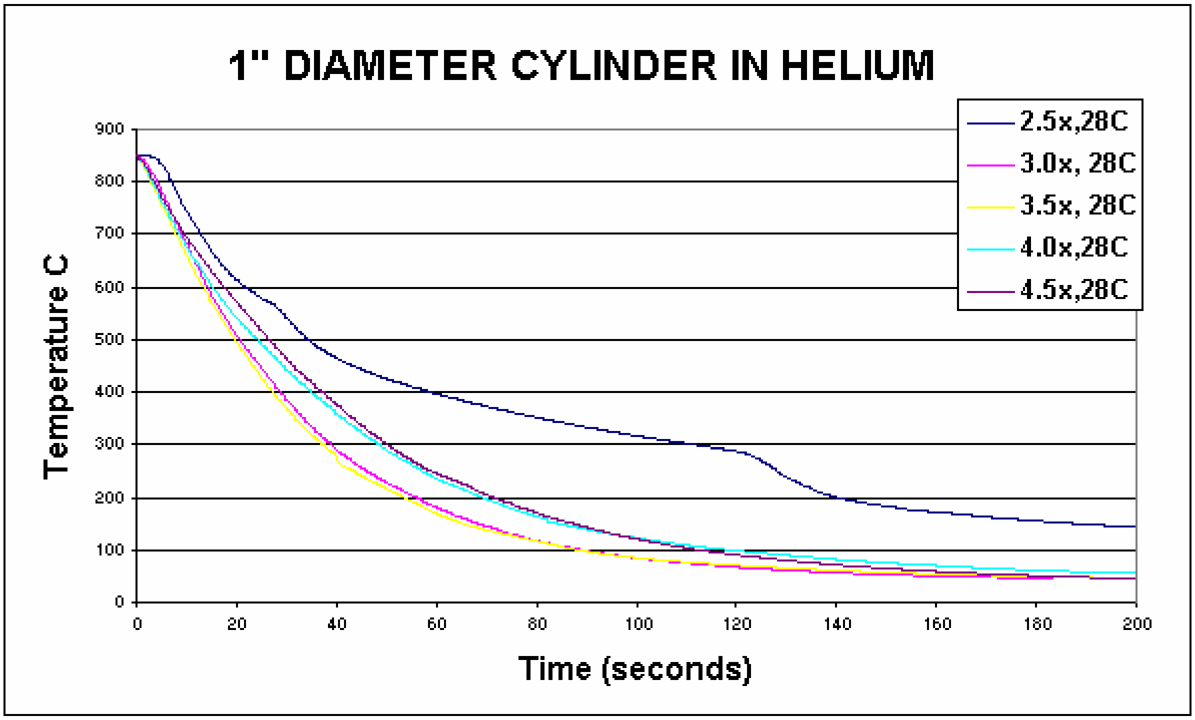

Figure 2. Cooling curves measured for 1" diameter probes of stainless steel 304 in helium.

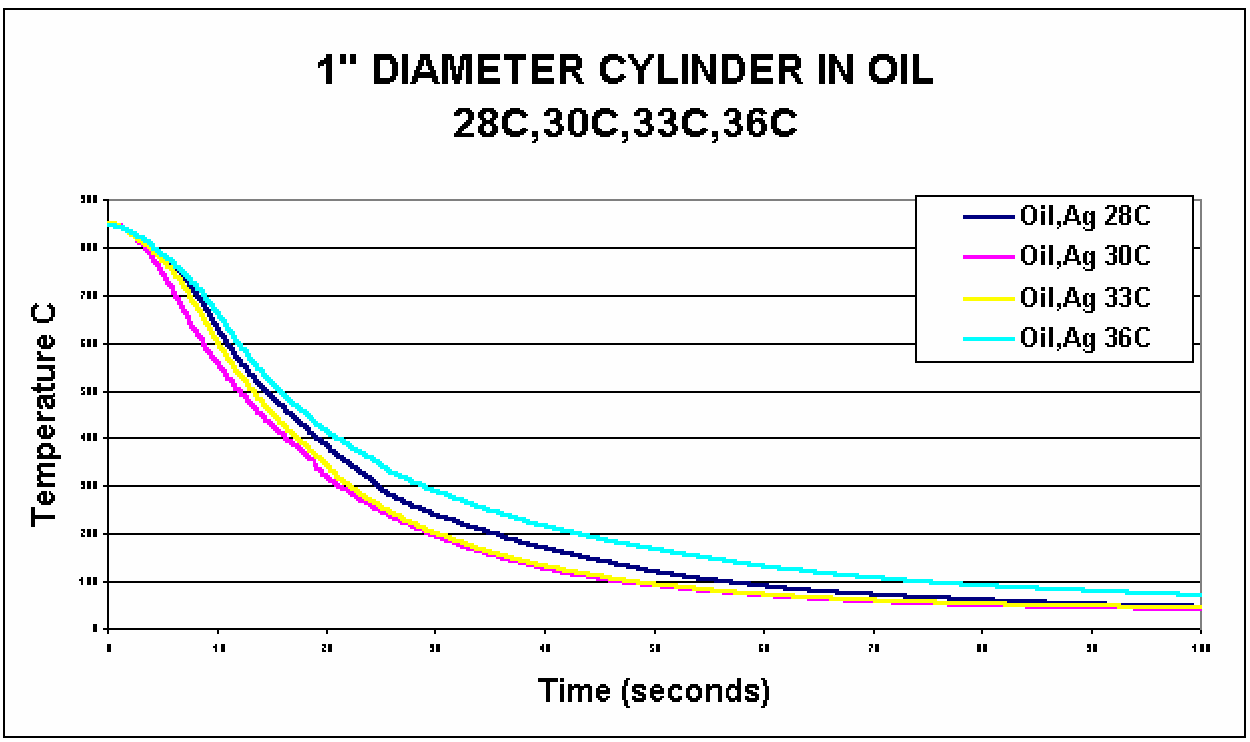

Figure 3. Cooling curves measured for 1" diameter probes of stainless steel 304 in oil at different temperatures.

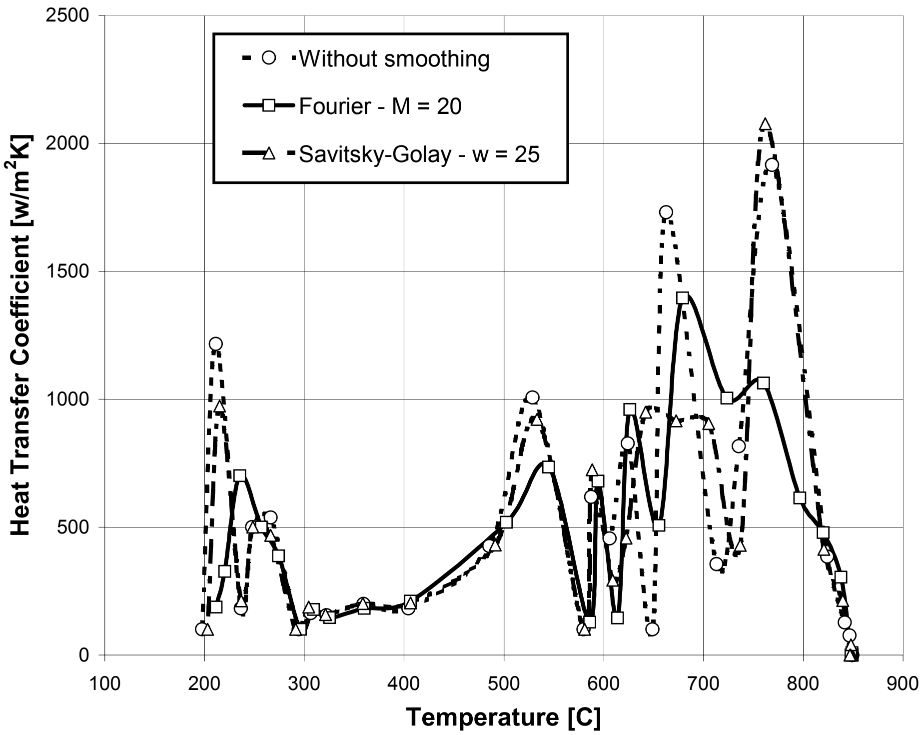

Figura 4: Heat transfer coefficient calculated for the probe 2.5x, 28℃, using the original cooling curves and the resultant ones of smoothing by the Savitzky–Golay algorithm (with w = 25) and the Fourier technique (with M = 2).

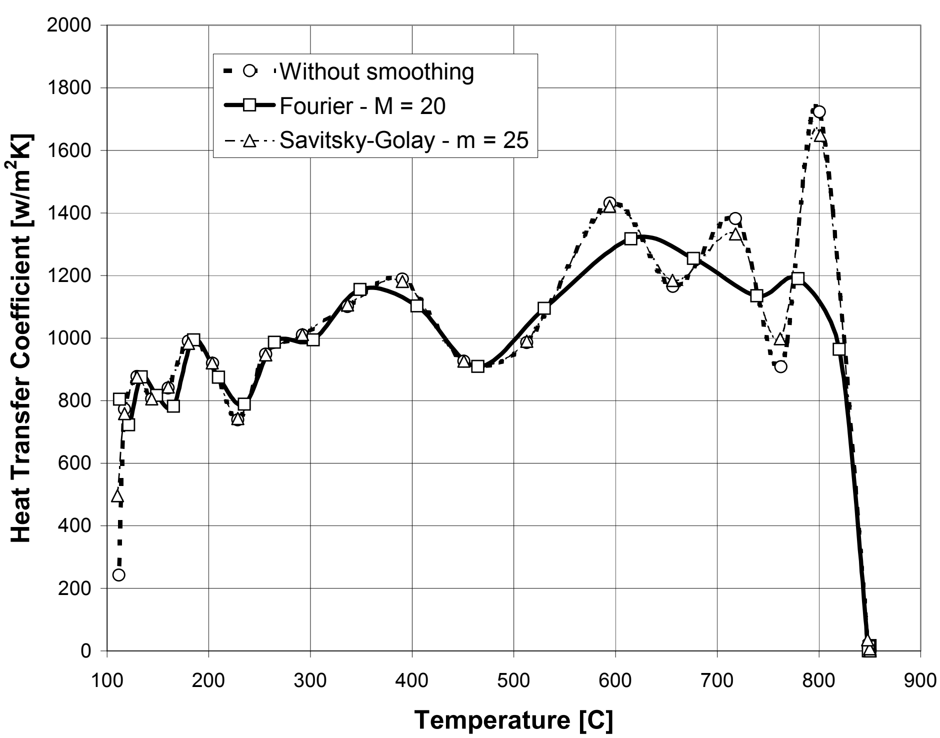

Figura 5: Heat transfer coefficient calculated for the probe 3.0x, 28℃, using the original cooling curves and the resultant ones of smoothing by the Savitzky–Golay algorithm (with w = 25) and the Fourier technique (with M = 2).

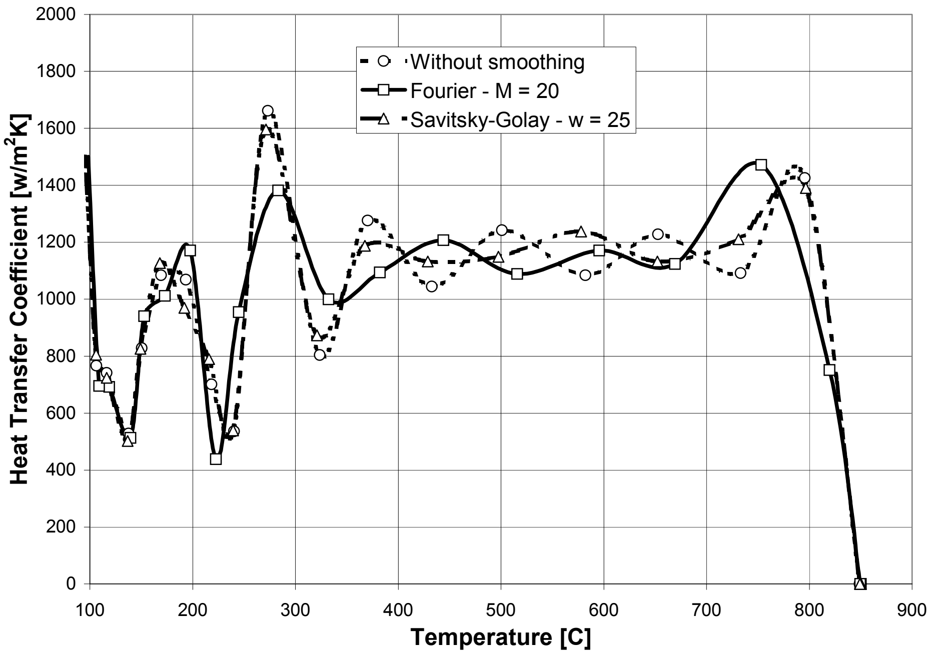

Figura 6.- Heat transfer coefficient calculated for the probe 3.5x, 28℃, using the original cooling curves and the resultant ones of smoothing by the Savitzky–Golay algorithm (with w = 25) and the Fourier technique (with M = 2)

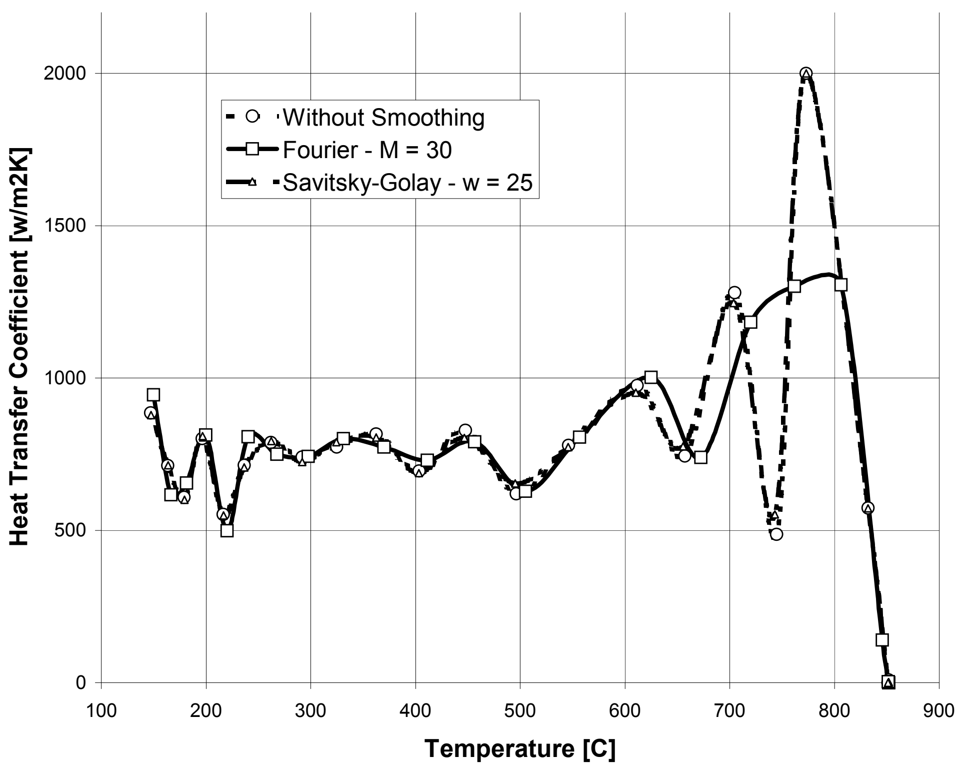

Figura 7.- Heat transfer coefficient calculated for the probe 4.0x, 28℃, using the original cooling curves and the resultant ones of smoothing by the Savitzky–Golay algorithm (with w = 25) and the Fourier technique (with M = 30)

Results of the simulations and conclusions

INC-PHATRAN Code was used to calculate the temperature dependent heat transfer coefficient corresponding to the 9 heat treated probes whose cooling curves are shown in figures 2 and 3. Values of the thermal conductivity and the specific heat as depending of the temperature, and of the density, assumed for the probe material (Stainless Steel 304) are indicated in Table 1. The smoothing Fourier technique with M = 20, 30, 40 and 50 was applied to each one of the cooling curves, and the corresponding HTC was also calculated by INC-PHATRAN. For comparison, the Savitzky – Golay algorithm with n_R = 5, 11, 15, 17, 21 and 25 was also applied to all the cooling curves, and the same analysis with INC-PHATRAN are also performed.

Table 2 shows the mean quadratic difference between the time-dependent temperature measured by the thermocouples (or the smoothed curves), and the temperature at the place of the thermocouple obtained by simulation with INC-PHATRAN after the optimization of the heat transfer coefficients was performed, for each one of the cases analyzed.

Some comparisons of the heat transfer coefficients obtained using the original cooling curves and the smoothed ones by the Fourier technique are shown in figures 4 to 7. The results obtained after smoothing cooling curves with the Savitzky – Golay algorithm are also included in the graphs. Great enhancements of the oscillations in the HTC typically produced by noise in the cooling curves, are evidently achieved with the use of the Fourier smoothing technique.

Acknowledgements

The authors thank the support given by Universidad de Buenos Aires, Argentina, through the Grant UBACYT TI035 (1998-2000).

References

1. G.E. Totten, M.E. Dakins and R.W. Heins "Cooling Curve Analysis of Syntetic Quenchants - A Historical Perspective", *Journal of Heat Treatment*, *6* (1988), pp. 87-95
2. M.E. Dakins, G.E. Totten and R.W. Heins "Cooling Curve Shape Analysis Can Help Evaluate Quenchants", *Heat Treating*, 12 (1988), pp. 38-39.
3. J.V. Beck, B. Blackwell and C.R.ST. Clair Jr., "Inverse Heat Conduction, Ill-posed Problems", John Wiley & Sons, New York, 1985.
4. R. Annino, R.D. Driver: "Scientific and Engineering Applications with Personal Computers", John Wiley & Sons, New York, (1986).
5. I. Felde, T. Reti, and X.L. Chen: "Efficient Data Eding and Filtering for Quenching Analysis". *The 3rd International Conference on Quenching and Control of Distortion*, Prague, Czech Republic, 24-26 March 1999. Pp. 208-215.
6. G. Sánchez Sarmiento and C. Barragán, "INC-PHATRAN: A computer model for the simulation of heat-treating processes, User manual", SOFT-ING Consultores, April 1997.
7. G. Sánchez Sarmiento, A. Gastón and J. Vega: "Inverse heat conduction coupled with phase transformation problems in heat treating process". *E. Oñate and S.R. Idelsohn, Eds.: COMPUTATIONAL MECHANICS - New Trends and Applications.* CIMNE, Barcelona, España, 1998. CD-Book. Part VI, Section 1, Paper 16.
8. G. Sánchez Sarmiento and J. Vega: "Calculation of the hardness space distribution in the as quenched condition of a medium hardening tool steel". *1st International Conference on Thermal Process Modeling and Computer Simulation*, Shanghai Jiao Tong University, Shanghai, China, March 28 – 30, 2000.
9. G. Sánchez Sarmiento, X.L. Chen, J. Vega, G.E. Totten, R. Raynoldson, L. Huynh and L. Meekisho: "A Comparison on Cooling Curve Analysis using Inc-Phatran and Winprobe". *The 20th Heat Treating Society Conference and Show*, St. Louis, Missouri, USA, October 9-12, 2000.