

## Trend analysis in the 1D solution of the inverse heat conduction problem by the sequential function specification technique

### Análisis de tendencia en la solución 1D de un problema inverso de conducción de calor por la técnica secuencial de especificación de la función

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#### Abstract

Inverse heat conduction problems are categorized by the solution technique or algorithm (Function Specification, Regularization, Laplace Transform, Conjugate Gradient, Mollification), by the solution method (Duhamel's Theorem, Difference Method Finite, Finite Element Method), and by the time domain (Stoltz Method, Sequential Method, and Complete Domain). In the direct approach, the unique solution of an effect due to a cause is obtained. From the cause-effect view, inverse problems are characterized by not meeting the existing criteria and the uniqueness of determining the cause when analyzing an effect. However, this has promoted the implementation of robust methods to optimize the stability of a solution. In this work, the study system consists of a long solid cylinder at an elevated temperature that is cooled. The implemented methodology allowed the creation of data trends through linear extrapolation to improve estimation accuracy for abrupt changes in the function (boundary condition). The results show an acceptable increase in punctual precision in the estimation, and it is a consequence of the solution that the calculated thermal histories already contain an implicit degree of error.

**Inverse problems, Heat transfer, Sequential function specification**

#### Resumen

Los problemas inversos de conducción de calor se categorizan por la técnica o algoritmo de solución (Especificación de la Función, Regularización, Transformada de Laplace, Gradiente Conjugado, Mollificación), por el método de solución (Teorema de Duhamel, Método de Diferencias Finitas, Método de Elemento Finito) y por el dominio de tiempo (Método de Stoltz, Método Secuencial y de Dominio completo). De la visión causa-efecto, a diferencia de un planteamiento directo en el que se obtiene la solución única de un efecto debido a una causa, los problemas inversos se caracterizan por no cumplir los criterios de existencia y unicidad de determinación de la causa cuando se analiza un efecto. Esto ha promovido la implementación de métodos para optimizar la estabilidad de una solución. En este trabajo el sistema de estudio consiste de un cilindro sólido largo a temperatura elevada que se enfría. La metodología implementada permitió crear tendencias de datos mediante extrapolación lineal para mejorar la precisión de estimación para los cambios abruptos de la función (condición de frontera). Los resultados obtenidos muestran un incremento aceptable de precisión puntual en la estimación, pero se induce por solución que las historias térmicas ya contienen implícito un grado de error.

**Problemas inversos, Transferencia de calor, Especificación secuencial de la función**

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## Introduction

The interest in the theory and application of inverse mathematical problems has maintained constant work since its growing use in the last century. The inverse problem statement is found in diverse applications of science and engineering, contributing to creating new paradigms in the field of research due to its unique characteristic of not having a single solution. This condition mathematically defines them as poorly conditioned problems; therefore, they generally require applying specific mathematical techniques to ensure the solution method's stability (Beck, Litkouhi, & St. Clair, 1982) (Krzysztof, 2011) (Meekisho, Hernandez-Morales, Tellez-Martinez, & Chen, 2005) (Beck, Blackwell, & Haji-Sheikh, 1996) (Blanc, Raynaud, & Chau, 1998). Therefore, since there is high-capacity computing technology, the possibility of implementing additional analyzes or modifications to the techniques that contribute to its optimization arises. In metallurgical processes that occur in transitory states of heat transfer, knowledge of the conditions that modify the thermal field of a system is vital to obtain better control.

In particular, heat conduction problems are a reference for the frequent application of the inverse formulation. Some examples are the nuclear, aerospace, mechanical, and metallurgical fields (Hernández-Morales, Cruces-Reséndez, & Téllez-Martínez, 2018) (Kumar, 2004). In metallurgical processes that occur in transitory states of heat transfer, knowledge of the conditions that modify the thermal field of a system is vital to obtain better control. Therefore, the formulation and solution of an inverse heat conduction problem (IHCP) will consider a viable method to achieve this.

This work shows the analysis of the behavior of the temperature change rate at a point near the border of a system. It can use to define critical points of the variation of the thermal boundary condition before estimating it by the sequential function specification (SFS) technique. This analysis was carried out to implement improvements in estimating thermal boundary conditions through trend analysis, and to define key points of extrapolation techniques from thermal history data obtained by direct measurement.

The results obtained help to propose the modification of the data trend in the thermal history to avoid losing precision in the characteristic biases of the estimated function; the subsequent calculation of the thermal field would introduce differences concerning the reference temperatures.

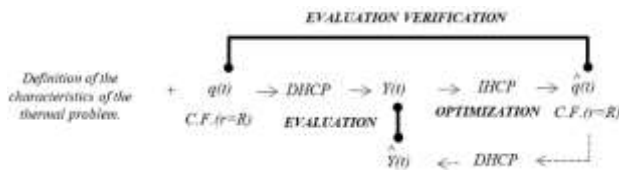
## Development

Precisely, the development of this work consists of proposing the mathematical model that governs heat transfer by conduction in a solid cylinder considered to be of infinite length (on its axial axis) and performing the following procedure:

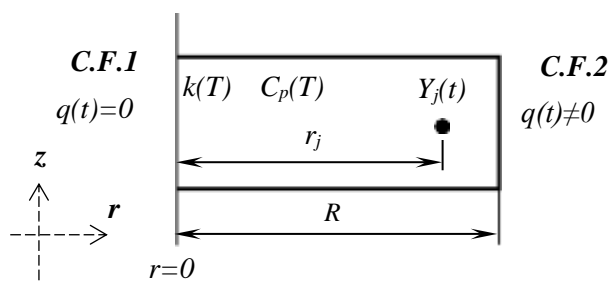
- a) Define the characteristics of the problem considering the interaction of the solid with a medium at different temperatures.
- b) Solve the forward heat conduction problem (DHCP) in a transient state by setting a known thermal boundary condition  $q(t)$ .
- c) Process at least one thermal history  $Y_j(t)$  calculated in the vicinity of the surface of the solid in contact with the medium.
- d) Solve the inverse heat conduction problem (IHCP) using the thermal history(s) from the previous step to estimate the thermal boundary condition  $\hat{q}(t)$ .
- e) Validate the mathematical model using the results obtained in the previous step by evaluating the differences (error) between the proposed and estimated thermal boundary conditions and the thermal histories. In particular, the thermal history  $\hat{Y}_j(t)$  is equivalent to the one processed in step (c).
- f) Carry out the steps from (a) to (e) introducing the optimization method.

Fig. 1 schematically summarizes the previous procedure, and Fig. 2 outlines the characteristics of the thermal problem considering a representative element of the system under study.  $Y(t)$  represents the known thermal history,  $r$  and  $z$  represent the geometric variables, radius, and length, respectively, as well as  $k(t)$  and  $C_p(t)$ , the thermal conductivity and thermal capacity of the material, respectively.

The maximum dimension of the element radius will specify with the magnitude  $R$ , and  $r_j$  represents the position concerning the cylinder center of the thermal history(s) used for the analysis of the IHCP as a function of the value of indicator  $j$ . The material's properties depend on the temperature  $T$  for the approach in this work.



**Figure 1** Schematic procedure for the development of data generation and its analysis. Source: *Self-Made [MS Word LTSC Pro Plus 2021]*



**Figure 2** Schematic representation of the axisymmetric element of the system under study and the characteristics of the thermal problem

Source: *Self-Made [MS Word LTSC Pro Plus 2021]*

The mathematical formulation of DHCP that governs the transfer is:

$$\frac{1}{r} \frac{\partial}{\partial r} \left( kr \frac{\partial T}{\partial r} \right) = \rho C_p \frac{\partial T}{\partial t}, \quad 0 \leq r \leq R, \quad t > 0 \quad (1)$$

$$\frac{\partial T}{\partial r} \Big|_{r=0} = 0, \quad -kr \frac{\partial T}{\partial r} \Big|_{r=R} = q(t) \quad (2)$$

$$T(r, T) = T_0, \quad 0 \leq r \leq R, \quad t > 0 \quad (3)$$

Where  $\rho$  represents the density of the material as a constant property. On the other hand, the IHCP approach is formulated similarly to DHCP with changes in equations (2) and (3), such that:

$$\frac{\partial T}{\partial r} \Big|_{r=0} = 0, \quad -kr \frac{\partial T}{\partial r} \Big|_{r=R} = q(t) = i? \quad (4)$$

$$T_j = (r_j, t_i) = \hat{Y}_j, \quad j = 1, 2, \dots, n, \quad i = 1, 2, \dots, M \quad (5)$$

Where  $i$  represents the number of elapsed time steps or time index until the current calculation step  $M$  in the temporal analysis interval of the thermal phenomenon.

It was to use the SFS technique to solve the IHCP. In the technique, the sum of the squares of the difference between the measured temperatures  $Y_j$  and the estimated temperatures  $\hat{Y}_j(t)$  is minimized in a calculation time interval  $(M + l - 1)$  to estimate at the same time the thermal boundary condition as a function of known thermal histories ( $j = 1, 2, \dots, n$ ). The objective function defines as:

$$\frac{\partial S}{\partial q} = \frac{\partial}{\partial q} \left[ \sum_{l=1}^L \sum_{j=1}^n (Y_{j, M+l-1} - \hat{Y}_{j, M+l-1})^2 \right] = 0 \quad (6)$$

Where  $l$  is the index that defines the number of discrete temperature data at time instants after calculating instant  $M$ . This index is called the future time step index. It establishes that the solution is "stabilized" for estimating the thermal boundary condition that satisfies the energy balance in the mathematical heat conduction model. Therefore, when developing equation (6), it is established that the sequential estimation of the boundary condition can obtain it through the following equation:

$$q_M = q_{M-1} + \frac{1}{\Delta M} \left[ \sum_{l=1}^L \sum_{j=1}^n (Y_{j, M+l-1} - \hat{Y}'_{j, M+l-1; q})^2 \right] (\hat{Y}'_{j, M+l-1; q}) \quad (7)$$

The apostrophe means the calculation of the field variable considering the properties that prevail in the conditions of the calculation step  $(M - 1)$ . That is, at the instant prior to estimating the boundary condition value. In this way,  $\hat{Y}'_{j, M+l-1; q}$  represents corresponding values of the field variable called sensitivity coefficient, defined by the differentiation of equations (1) to (3) concerning the estimated variable  $q$ .

$$\Delta M = \sum_{l=1}^L \sum_{j=1}^n (\hat{Y}'_{j, M+l-1; q})^2, \quad \hat{Y}'_{j, M+l-1; q} = \frac{\hat{Y}_{j, M+l-1}}{\partial q_M} \quad (8)$$

As part of the thermal problem analysis procedure, a computer program written in Visual C# language was generated to solve both DHCP and IHCP.

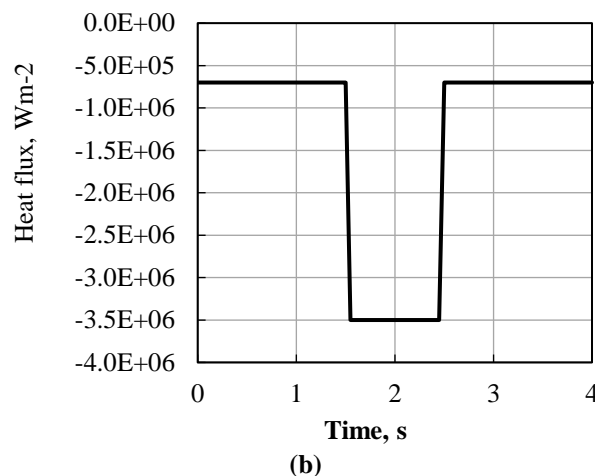
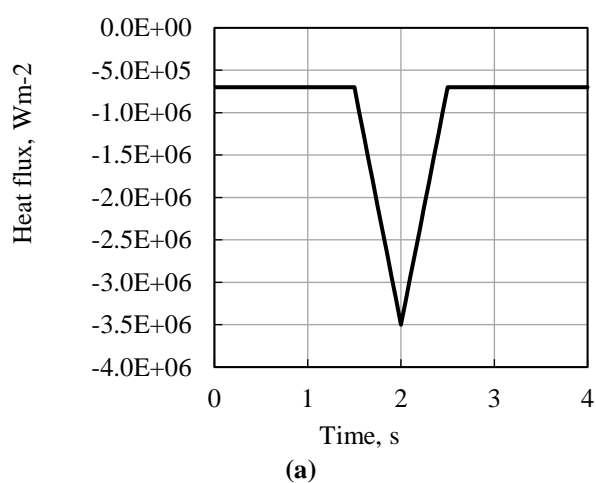
The DHCP solution was verified with results obtained from generating various models in the Ansys® commercial program, which establishes a high degree of confidence in the results of the IHCP solution.

In particular, the methodology adopted for the analysis considers the cooling of the cylinder element from an initial temperature of 911°C. The thermal properties used were obtained from the literature and correspond to AISI 304 stainless steel. The traces of the thermal boundary conditions used are shown in the graphs of Graphic. 1(a) and 1(b).

## Results and Discussion

According to the procedure described at the beginning of the preceding section and outlined in Fig. 1, the thermal boundary conditions  $q(t)$  was used to solve the DHCP using the Ansys computer program. In the analysis, an axisymmetric model with a radius  $R=0.635$  mm defined, creating a partition of the section drawn at 1 mm from the surface. First-order quadrilateral finite elements were used in the structured mesh type, defining 10 and 20 elements in the sections 1 mm and 0.535 mm.

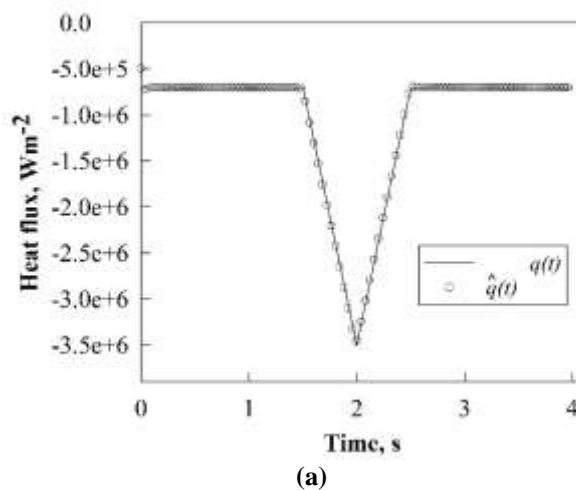
Thermal history calculations with a step of 0.01 at the partition position were used to solve the IHCP using the computer program developed for this work. The algorithm proposed the finite difference technique through the Crank-Nicolson solution method and the Thomas method for the inversion of the matrix of the system of equations. The program was subjected to a mesh sensitivity analysis, determining that ten control volumes in both sections, considering the same system partition, are adequate to obtain results without discretization effects.

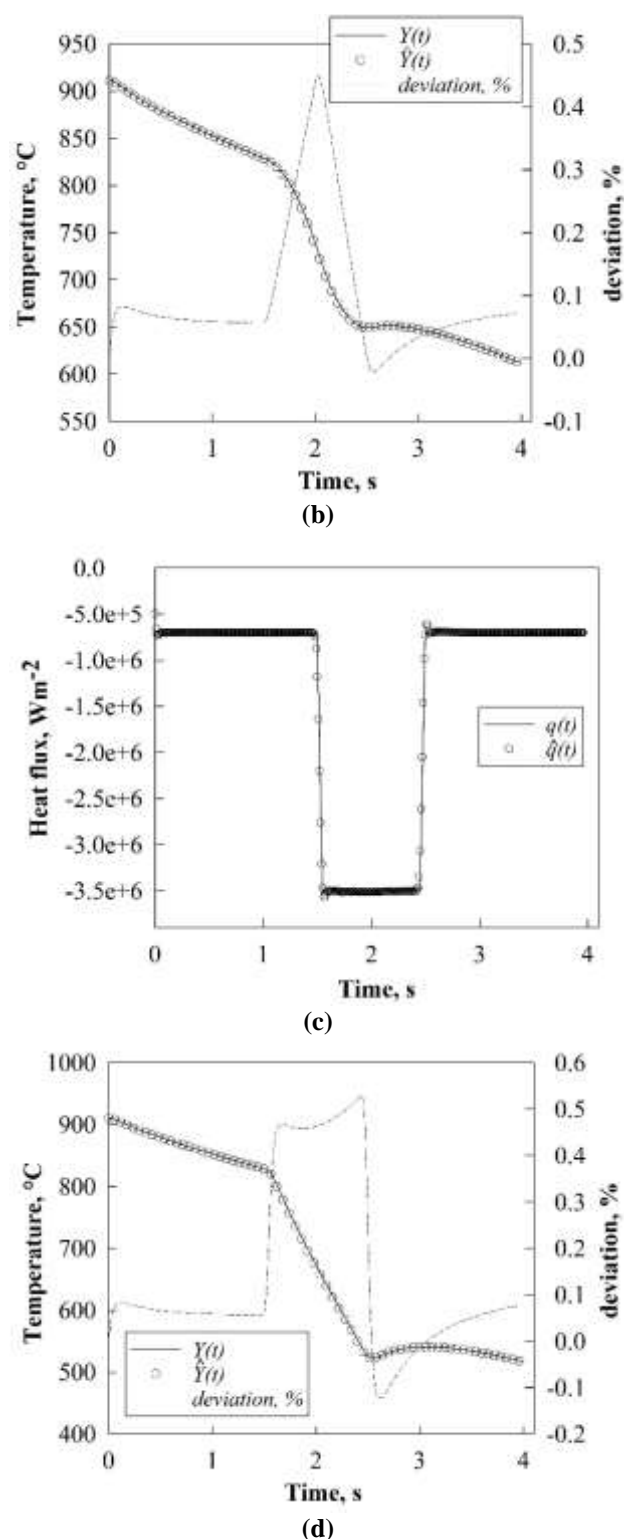


**Graphic 1** Graphical representation of the functions  $q(t)$  (thermal boundary conditions) proposed for the cases of thermal analysis

Source: Self-Media [MS Excel LTSC Pro Plus 2021]

The results of the estimation of the thermal boundary conditions product of the IHCP solution using several future time steps  $L=4$ , as well as the thermal histories calculated after solving the DHCP, with the respective ones, are shown. Graphic 2. The curves drawn with solid lines represent the reference data, and those drawn with symbols represent the estimates (specifying the comparison step associated with virtual validation). Additionally, graphs (b) and (d) show curves with segmented lines that indicate the temperature data's deviation percentage. The deviation is less than 1%, indicating that even with the abrupt changes and magnitudes of the boundary conditions in each case, the IHCP solution generates excellent results. Analyzing the deviation percentage curves (segmented line of graphs (b) and (d) of graphic 2), it can be deduced that the temperature variations resemble in segments the functional form of the heat flux density curve.



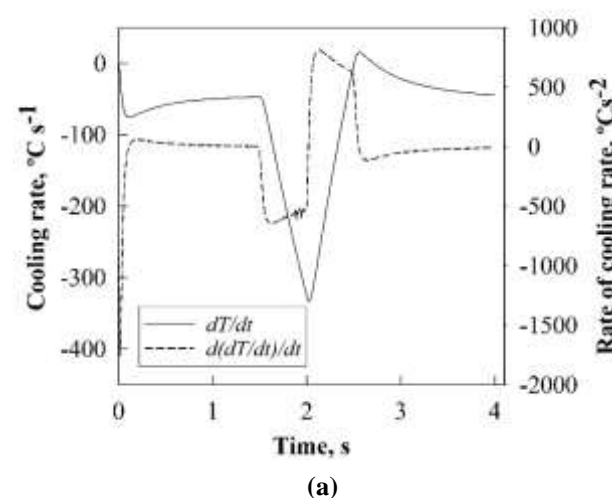


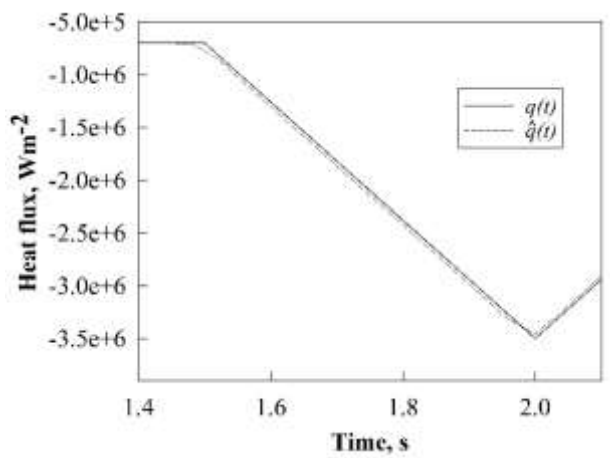
**Graphic 2** Graphs (a) and (c): curves of the proposed thermal boundary conditions  $q(t)$  (continuous line) and estimated  $\hat{q}(t)$  solving the IHCP (open symbols). The curves of graphs (b) and (d) show the excellent validation of the calculated thermal histories  $\hat{Y}(t)$  (open symbols) and the reference  $Y(t)$  (continuous line) in each case of the proposal. The dashed line shows the % deviation. Source: Self-Made [SigmaPlot V12.0]

Thus, if in the transient heat transfer state, the thermal field is affected by the rate of change of the thermal boundary condition, then the rate of temperature must reflect the same critical values of the differences between the reference and calculated thermal history.

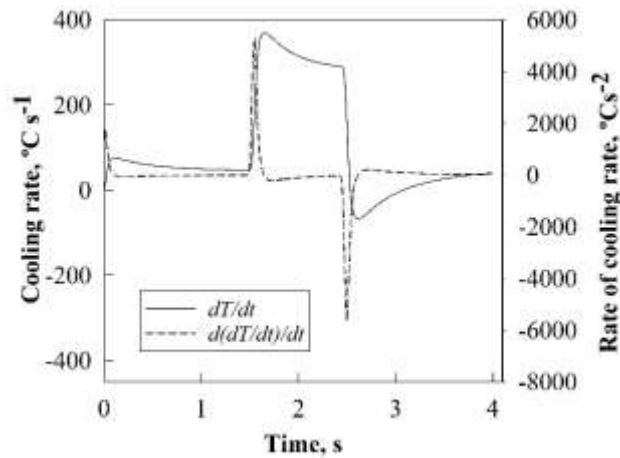
Graphic 3 shows the cooling rate curves' calculation, and the rate of change thereof in graphs (a) and (c) for each case analyzed. The results make evident the similarity of the behavior of the cooling rate and the percentage deviation curve, while the curves of the rate of change of the cooling rate precisely define the points of critical changes in the thermal boundary condition. That is, in small changes in cooling rate, the rate of change is close to zero. While being significant, they deviate towards negative or positive values depending on the increase or decrease in cooling rate, respectively. On the other hand, manipulating the scale in graphs (b) and (d) allows us to note the deviations from the estimated boundary condition.

Defining the critical points to implement a possible correction in the calculation process is essential. The deviation in the estimate starts at the first critical point of the cooling rate due to the SFS technique. The greater the number of temperatures considered, the more significant the deviation, which depends on the number of future temperatures that are considered to solve the objective function at each time step (refer to Eq. 6). In an attempt to correct the deviation in the first abrupt change for the proposed functions, the analysis of the trend of the data, both of the boundary conditions and the reference thermal histories, was carried out to accurately determine the point critical variation of the rate of cooling. The point in question was found at a time of 1.47 s. According to this reference, it is observed that to estimate the function data; it is necessary to modify the trend of the thermal history, adopting a linear behavior from 1.46 s, that is, keeping the cooling rate before the critical deviation. The extrapolation curve and usual trend are shown in Graphic 4, considering that four data are used for the SFS technique in the IHCP solution.

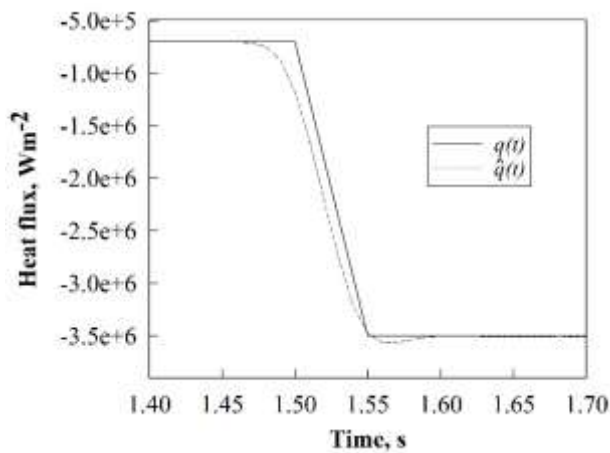




(b)



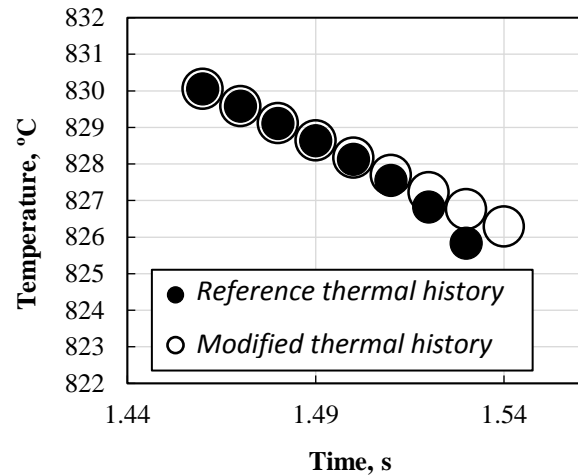
(c)



(d)

**Graphic 3** Graphs (a) and (c) show the cooling rate curves (continuous line) and their rate of change (dotted line) concerning the reference thermal history  $Y(t)$  for each case studied. The deviations of the estimated boundary condition  $\hat{q}(t)$  concerning those proposed  $q(t)$  are exemplified by plotting the curves at a modified scale in graphs (b) and (d)

Source: Self-Made [SigmaPlot V12.0]



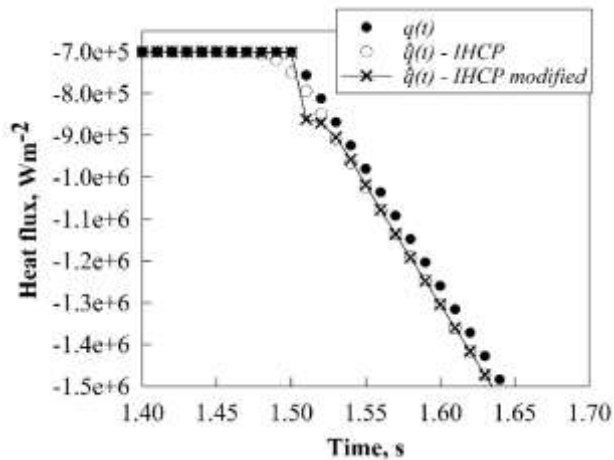
**Graphic 4** Reference thermal history (closed symbols) and modified thermal history (open symbols) curves, respectively. The second is created by extrapolation to force the temperature field calculation at the critical point of the thermal boundary condition

Source: Self-Made [MS Excel LTSC Pro Plus 2021]

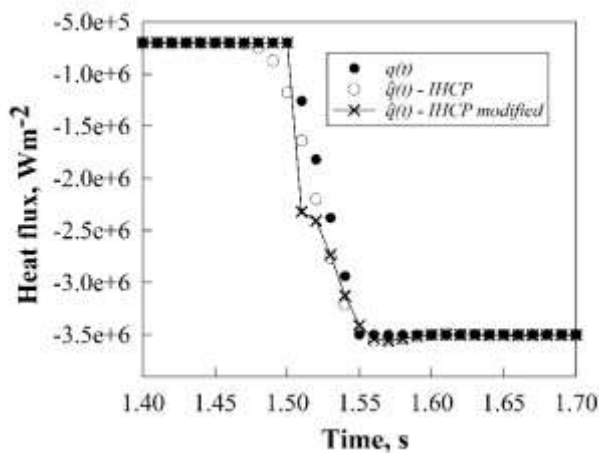
Additionally, graphs (a) and (b) of Graphic 5 also show the curves of the functions proposed (closed symbols) and estimated with and without the implementation of the modification by extrapolation (open symbols and line with symbols in x). It can be seen in both cases that the modified solution adjusts excellently to the point of change of direction at 1.5 s. Notwithstanding, the stability of the solution is lost when calculating the value of the functions in 1.51 s. For this point, the modification with extrapolation is no longer used, and although the function recovers its original trend, continuity on the curve of the proposed function is not achieved.

Through the analysis of the obtained information set, it can be deduced that starting from virtually constructed information, the modification of the estimated function will not depend on the optimization of the objective function (refer to Eq. 6).

The angular form of the proposed boundary condition function has not been strictly applied in the DHCP solution. Although there is an error in the IHCP solution, as indicated by the temperature differences (refer to graphs (b) and (d) of graphic 2), the reference thermal histories already introduce a certain degree of deviation from the numerical solution of the direct model.



(a)



(b)

**Graphic 5** Plots (a) and (b) show, at a fraction of a scale, the curve comparison of the proposed (closed symbols), modified estimated (line and symbols), and estimated (open symbols) heat flux density functions by solving the IHCP

Source: Self-Made [SigmaPlot V12.0]

## Thanks

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## Conclusions

Considering that temperature-dependent thermal properties were used for the thermal analysis, the validation results of the IHCP have a low degree of uncertainty. The approach of the case studies free of systematic errors allows us to determine that the SFS technique can be optimized through a trend analysis coupled with the stability introduced by the number of future time steps.

On the other hand, the defined analysis procedure will support the study of analytical systems to have better control of the reference information and those influenced by systematic errors (noise) with more than one active thermal boundary condition.

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