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A NONLINEAR INVERSE HEAT CONDUCTION TECHNIQUE TO ESTIMATE THERMAL PROPERTIES OF METALS

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Abstract. *This work presents a nonlinear inverse heat conduction problem technique to estimate simultaneously the thermal conductivity, k, and volumetric heat capacity,* ρc_p*, temperature-dependent of an AISI 304 stainless steel sample. The thermal model is based on a transient one-dimensional heat diffusion equation, with constant and uniform heat flux applied on the top surface and an insulation condition on the bottom. The heat flux intensity, duration of the experiment, interval of data acquisition and others were determined through the analysis of the sensitivity coefficients. To estimate the thermal properties, an iterative technique for nonlinear inverse problems, based on the Gauss method of minimization with regularization for future times was applied. The simultaneous estimation depends on the definition of an objective function, determined by the squared difference of the experimentally simulated and numerical temperatures. The solution of the heat diffusion equation by the Finite Difference method with implicit formulation provides the numerical temperature, and the simulated experimental temperature is obtained by the addition of residuals to the numerical data. The estimated properties presented a good agreement when compared with literature.*

Keywords: *heat conduction, simultaneous estimation, thermal conductivity, volumetric heat capacity, nonlinear problem.*

1. INTRODUCTION

Discovered in prehistory, metallic materials and his several functionalities have provided a series of social chances. As knowledge of metallurgy has developed, metals have played an important role in the expansion of nations, growth of agriculture, commercial activities, transports and craft. Since then, metals have become part of the most varied aspects of life, being fundamentals throughout the industry. Their large applicability motivated studies, development and adaptation of these materials, looking for properties increasingly appropriate to the needs experienced. An essential part of this process, the determination of thermophysical properties are fundamental in the characterization of their behavior regarding temperature variations.

Allied to the mathematical modeling, the use of numerical methods made it possible to make predictions of the behavior of a body under the most varied circumstances. For this purpose, it is essential to know geometry, physical parameters and initial and boundary conditions. However, if some of these variables are unknown or impossible to be directly obtained, it is necessary to apply optimization techniques for the problem resolution.

These situations are common engineering problems. They can be found in processes as machining, welding, casting, forging, and others, in which the temperature control is extremely important and influenced mostly by the nature of the materials. In these processes, both the raw materials and the tools and accessories are under high temperature variations, so it is desirable that their properties are known in all ranges of operation. Therefore, thermal properties estimation is directly inserted in industry and its necessity increases allied to the development of new materials. It has contributed to the complete characterization of the material and allows correct application, in order to avoid failures, reduce costs and prolong life of components.

Representing, respectively, the amount of heat a material can transport and its capacity to store thermal energy, two essential properties in this context are thermal conductivity, *k*, and volumetric heat capacity, ρc_p. Over the years, several techniques have been developed in order determine these thermal properties in an increasingly effective way. Among them, three classical techniques stand out: the Hot Wire method proposed by Blackwell (1954), the Flash method developed by Parker *et al.* (1961) and the Guarded Hot Plate method normalized (ABNT, 2005). In these tasks, and generally in parameter estimation problems, such properties have been considered constants and determined for low or short heat intensities. In the last decades, however, interest in the estimation of these properties as functions of the temperature has increased.

Fundamental contributions have been made at the end of the last century (Özisik, 1993, Dowding *et al*., 1995, Sawaf *et al*., 1995, Yang, 1999). Woodbury (2003) presented several techniques for solving these problems, bringing together the detailed discussion of sequential parameter estimation method. This method is a tool of great importance in nonlinear problems, and has been subsequently used by several authors (Thomson, 2005, Zueco and Alhama, 2007, Mohamed, 2008). On the other hand, employing a different approach, Tillmann *et al.* (2008) and Carollo *et al.* (2019) adopt constant properties and estimate them within different temperature ranges. In addition, nowadays, more robust artificial intelligence algorithms have been widely used to determine these properties (Czél *et al*., 2014, Sun *et al*., 2018, Tariq *et al*., 2020).

In this work a nonlinear inverse heat conduction problem technique is presented in order to estimate simultaneously and sequentially the thermal conductivity, k, and volumetric heat capacity, ρc_p, as functions of temperature in a sample of AISI 304 stainless steel. The thermal model is based on a transient one-dimensional heat diffusion equation, with constant and uniform heat flux applied on the top surface and insulation condition on the bottom. The sensitivity coefficients have been analyzed to provide the thermal estimation. To estimate the thermal properties, an iterative technique for nonlinear inverse problems is applied, based on the Gauss method of minimization with regularization for future times (Beck and Arnold, 1977). The simultaneous estimation depends on the definition of an objective function, determined by the squared difference of the numerical and simulated temperatures. The solution of the heat diffusion equation by the Finite Difference Method (FDM) with implicit formulation provides the numerical temperature, and the simulated experimental temperature is obtained by the addition of residuals to the numerical data.

2. METHODS

2.1 Thermal model

The layout of the thermal model is presented in Fig. 1. It consists of a flat, homogeneous and square section sample, subject to the initial temperature, T_0, and transient heat flux ϕ (t) imposed by a resistive heater on the top surface. The whole set is involved by insulating material.

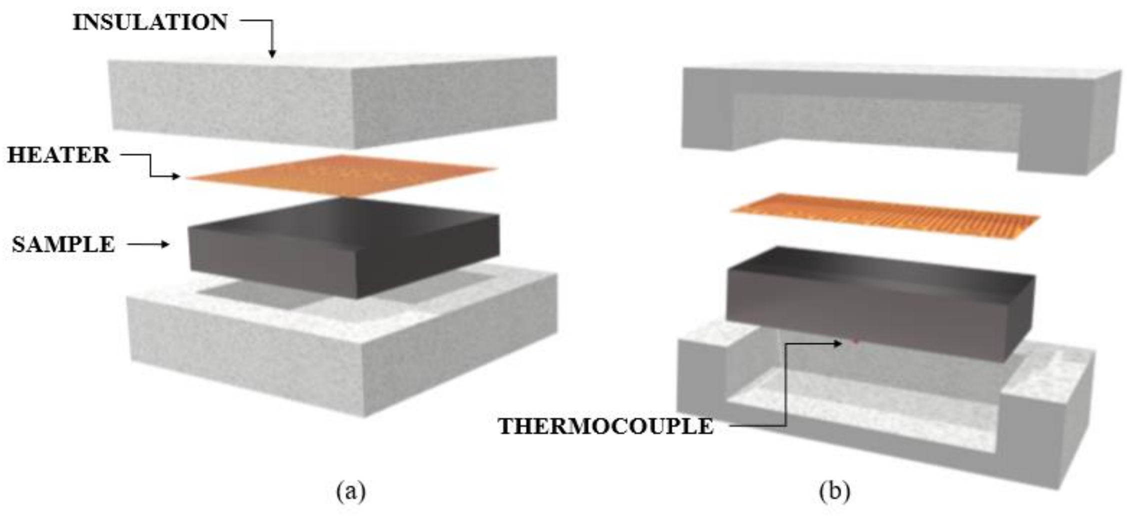


Figure 1. (a) Three-dimensional representation of the thermal model and (b) cross-sectional view.

To guarantee the unidirectional heat flux, as shown in Fig. 2, the analyzed sample has much smaller thickness, L, compared to the other dimensions. It is also considered that the sample and the heater have the same square section, promoting homogeneous heating over the entire surface.

The heat diffusion equation for this situation is given by:

$$\frac{\partial}{\partial x} k(T) \frac{\partial T(x,t)}{\partial x} = \rho c_p(T) \frac{\partial T(x,t)}{\partial t} \quad (1)$$

Subjected to the boundary conditions:

$$-k(T) \frac{\partial T(x,t)}{\partial x} = \phi(t) \qquad \text{at } x = 0 \quad (2)$$

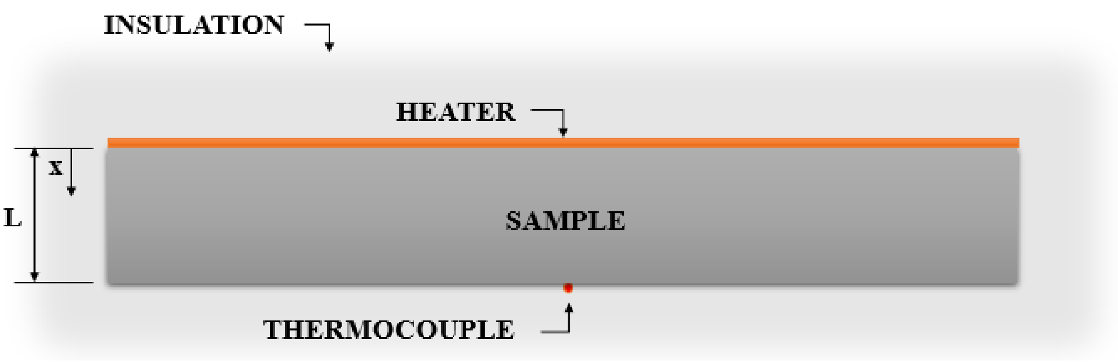


Figure 2. One-dimensional representation of the thermal model (cross-sectional view)

$$\frac{\partial T(x,t)}{\partial x}=0 \qquad \text{at } x = L \tag{3}$$

and with the initial condition:

$$T(x,t)=T_0 \qquad \text{at } t = 0 \tag{4}$$

where x is the Cartesian coordinate and t is the time.

2.2 Model solution

The numerical data is obtained through the discretization of the thermal model using FDM with implicit formulation. The method enables the determination of temperature at discrete points. Each point represents a certain region, and its temperature is a measure of the average temperature of the region. The Finite Difference method has been successfully used to solve one-dimensional heat conduction problems. Then, in a way to achieve temperature information as close as possible to real experimental data is computed by adding random error to the FDM numerical temperature.

Its choice is due to the fact that the implicit formulation does not have stability criteria, behaving satisfactorily for any time interval, Δt, imposed on the study. Moreover, it presents low computational cost and good results when solved by the Gauss-Seidel method.

The system of nonlinear equations resulting from the application of the FDM for all internal points of the mesh and from the discretization of the boundary conditions can be solved by an iterative process involving two levels. At the external level the system is linearized calculating the thermal properties with the temperatures obtained in a previous iteration. On the inner level the linearized system of equations is solved by the iterative method.

The Gauss-Seidel algorithm allows the use of temperatures calculated for previous times in the calculation of the current one. That allows each equation to be solved individually and makes it necessary to adopt a convergence criterion that minimizes the procedure errors. In this work, each new iteration is only performed when the difference between the current and previously calculated temperature, at the same point, is smaller than a predetermined error of approximately 10^{-10}.

2.3 Sensitivity coefficients

The quality of the thermal property estimation depends largely on how sensitive the system is to its variations. For this reason, criteria is established for analysis and the determination of optimal process conditions. In the present work, such analysis is performed by calculating the sensitivity coefficients defined as the first partial derivative of temperature in relation to the parameter P to be estimated (k and ρc_p), as follows:

$$X_{P_j}=P_j\frac{\partial T}{\partial P_j} \tag{5}$$

where T is the numerically calculated temperature, P the parameter to be analyzed and j the counter of points in time.

In the analysis, conditions that maximize the coefficients are sought, since the greater their magnitude, the greater the reliability of the results. In this way, it is possible to determine the position of thermocouples, duration of the experiments, intensity of the heat flux and interval of application. Moreover, the behavior of these coefficients over time is an important issue. In order to guarantee the correct estimation, it is essential that they do not present linear dependence and that their magnitude is not widely different.

2.4 Thermophysical properties estimation

The thermal properties are simultaneously and sequentially estimated over the whole temperature field using an iterative method based on the Gauss method of minimization with regularization for future times. Thus, an objective function is described as the squared difference of a vector $\boldsymbol{Y}$ of experimental temperatures and a same length vector $\boldsymbol{T}$ of numerical temperatures obtained from FDM and dependent on a vector of unknown parameters $\boldsymbol{\beta}$, composed by the thermophysical properties of the material.

In order to determine the parameters that compose the vector $\boldsymbol{\beta}$, the method is used to minimize the following objective function:

$$S=\sum_{k=M}^{M+r-1}(Y_k-T_k)^2 \tag{6}$$

where, M is the time step, and r is the number of future times, which can also be written as:

$$S=(\boldsymbol{Y}-\boldsymbol{T})^T(\boldsymbol{Y}-\boldsymbol{T}) \tag{7}$$

Once such vectors are correspondents, the ideal values for the parameters searched are the ones that minimizes their difference and, therefore, the value of S.

Each iteration performed gives the properties, k^M and $\rho c_p{}^M$, corresponding to the current instant of time, t^M. The regularization of these results has been done using the concept of future times, in which it is temporarily assumed that the properties remain constant from the instant M until the next r future times.

To solve this nonlinear problem, an iterative technique based on the Gauss Minimization Method (Woodbury, 2003) is presented.

Whereas $\boldsymbol{b} = [k; \rho c_p]$, the value of $\boldsymbol{T}$ in $\boldsymbol{\beta}=\boldsymbol{b}+\Delta\boldsymbol{b}$ can be approximated by expanding into a Taylor series as:

$$\boldsymbol{T}|_{b+\Delta b} \approx \boldsymbol{T}|_b+\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{\beta}}\bigg|_b \Delta\boldsymbol{b} \tag{8}$$

The gradient coefficient in Eq. (8) is actually a $m \times p$ matrix of sensitivity coefficients:

$$\boldsymbol{X_\beta}=\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{\beta}}=\begin{bmatrix} \frac{\partial T_1}{\partial \beta_1} & \cdots & \frac{\partial T_1}{\partial \beta_p} \\ \vdots & \ddots & \vdots \\ \frac{\partial T_m}{\partial \beta_1} & \cdots & \frac{\partial T_m}{\partial \beta_p} \end{bmatrix} \tag{9}$$

Replacing $\mathbf{T}$ for $\boldsymbol{T}|_{\boldsymbol{b}+\Delta\boldsymbol{b}}$ in Eq. (7):

$$S= (\boldsymbol{Y}-\boldsymbol{T}/_{\boldsymbol{b}}+\boldsymbol{X_\beta}\Delta\boldsymbol{b})^T(\boldsymbol{Y}-\boldsymbol{T}/_{\boldsymbol{b}}+\boldsymbol{X_\beta}\Delta\boldsymbol{b}) \tag{10}$$

The derivative of Eq. (10) is forced to zero, resulting in:

$$\Delta\boldsymbol{b}=(\boldsymbol{X_\beta}^T\boldsymbol{X_\beta})^{-1}\boldsymbol{X_\beta}^T(\boldsymbol{Y}-\boldsymbol{T}/_{\boldsymbol{b}}) \tag{11}$$

Equation (11) is used to progressively improve an estimation for the vector $\boldsymbol{b}$ through the following iterative algorithm:

1. Choose a convergence criterion;
2. Begin with an initial value for $\boldsymbol{b}^n$;
3. Compute the vector $\boldsymbol{T}|_{\boldsymbol{b}}$;
4. Compute the matrix $\boldsymbol{X_\beta}$;
5. Use Eq. (18) to compute $\Delta\boldsymbol{b}$;
6. If the process converged, the desired solution is found. If not, update the $\boldsymbol{b}$ vector according to:

$$\boldsymbol{b}^{n+1}=\boldsymbol{b}^n+\Delta\boldsymbol{b}^n \tag{12}$$

7. Return to step 3 and repeat until converged.

As described in Woodbury (2003), the convergence in step 6 is sometimes difficult. One technique to assure it is to insist that each component of the vector $\boldsymbol{b}$ has a small chance relative to its own value. In other words, if there are m unknowns, assure that

$$\frac{\Delta \boldsymbol{b}_M}{\boldsymbol{b}_M} \leq \delta \tag{13}$$

For $M = 1, 2\ldots, m\text{-}r\text{-}1$.

However, as Aguiar (2012) highlighted, the convergence of the method still may fail and no longer generate a correct sequence of estimations depending on the initial guess. So, some conditions for the choice of the initial values must be imposed. The most important requires that its value must be sufficiently close to the actual parameters, requiring prior knowledge of the characteristics of the material under study. Cases in which there is no prior information, resorting to artificial intelligence algorithms to find the value of the first iterations may be a strategy.

2.5 Simulated experimental procedure

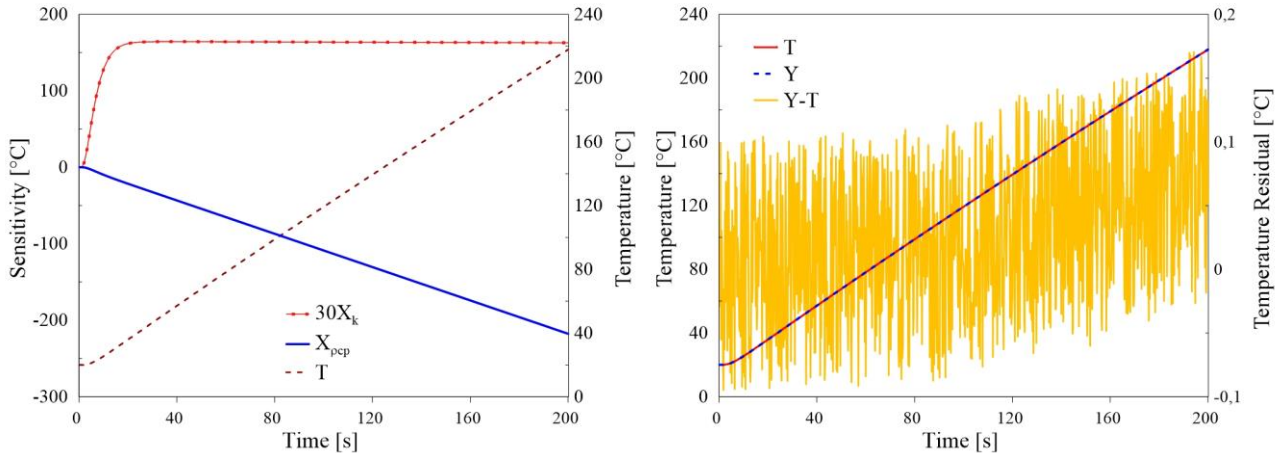
In the process of experimental data simulation, a flat and homogeneous AISI 304 stainless steel sample has been considered, with dimensions 50.0 mm x 50.0 mm x 10.1 mm. Its thermophysical properties were obtained from Carollo *et al*. (2019). A heat flux of 50.000 W/m² was imposed in 200 seconds, with initial temperature of 20°C. The interval for acquisition was considered 0.2 seconds for a thermocouple positioned on the opposite surface to the heating ($x=L$), respecting conditions that could be reproduced in laboratory. In order to reproduce a real experiment, the random errors added were of the order of ± 0.5°C, close to the uncertainty of a T type thermocouple.

3. RESULTS AND DISCUSSION

The sensitivity analysis aims to provide information about the viability of the estimation. For this purpose, the direct problem has been solved assuming, at first, constant properties. Figure 3(a) presents sensitivity coefficients at $x = L$, where the thermocouple is located. It is observed that X_k shows a fast growth and it stabilizes in the first seconds, assuming a constant value until the end of the simulation, similarly to the heat flux behavior. On the other hand, the absolute value of $X_{\rho cp}$ has a constant growth rate, proportional to the temperature variation. It is also clearly observed that the sensitivity curves have no dependence on each other, and both present good values along the experiment, therefore, the quality of the estimation is not affected.

Figure 3(b) presents the temperature variation through the simulated experiment in comparison to the numerical temperature calculated using FDM. In this case, thermal properties have been taken from the estimation. As it is shown, both temperatures have good agreement. Their difference is kept under 0.2°C, which is less than the uncertainty of a T type thermocouple and also less than the random errors added in the simulation, confirming the reliability of the method.

In addition, a mesh convergence study is accomplished for calculating the temperatures in both cases. Each mesh is considered to have a different number of elements (6, 8, 11 and 14) and even though the first two present some variations, meshes with 11 and 14 elements exhibit maximum temperature difference around 0.00058 °C. Thus, as both meshes presented practically the same results, in order to perform a lower computational cost, a 11-element mesh is employed. Moreover, when compared to temperatures obtained from COMSOL software with the same number of mesh elements, the difference remains under 10^{-6}.



(a) (b)

Figure 3. (a) Sensitivity Coefficients and (b) Numerical and Simulated Experimental Temperatures.

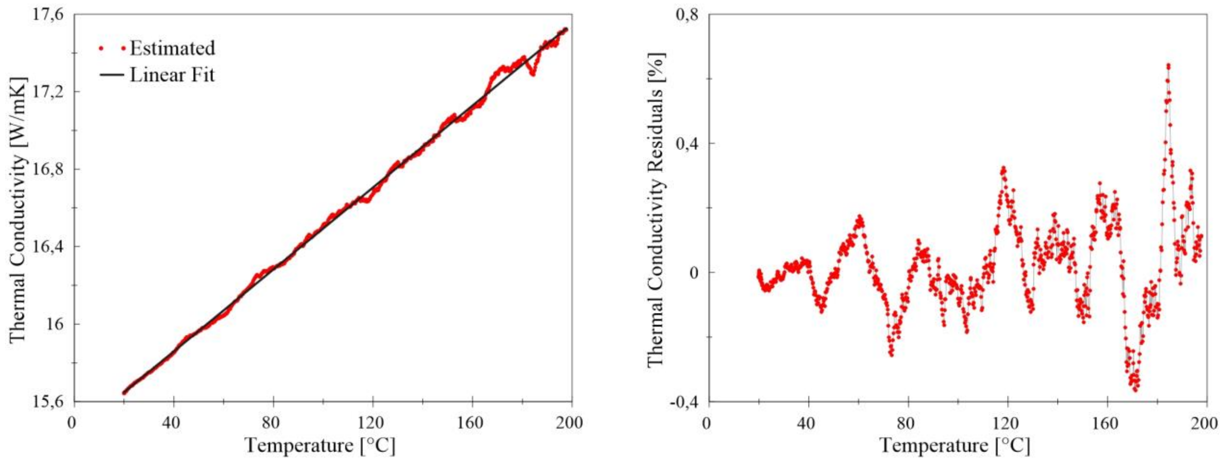
As it has already been highlighted, the initial guess for both parameters play an important role in the convergence of the method. To ensure the reliability of the results is recommended that, for each iteration, the initial guess must be around 0.5 and 1.5 times the true value. Therefore, in this study, for each estimation performed, the initial guess has been taken as the value of the property at room temperature taken from Carollo *et al.* (2019).

In the experimental simulation is considered that both thermal conductivity and volumetric heat capacity present linear variation with temperature, so results from the estimation are fitted through linear regression, expressed in Eqs. (14)-(15).

$$k(T)=0{,}01057\ T+15{,}4364\ \frac{\mathrm{W}}{\mathrm{mK}} \tag{14}$$

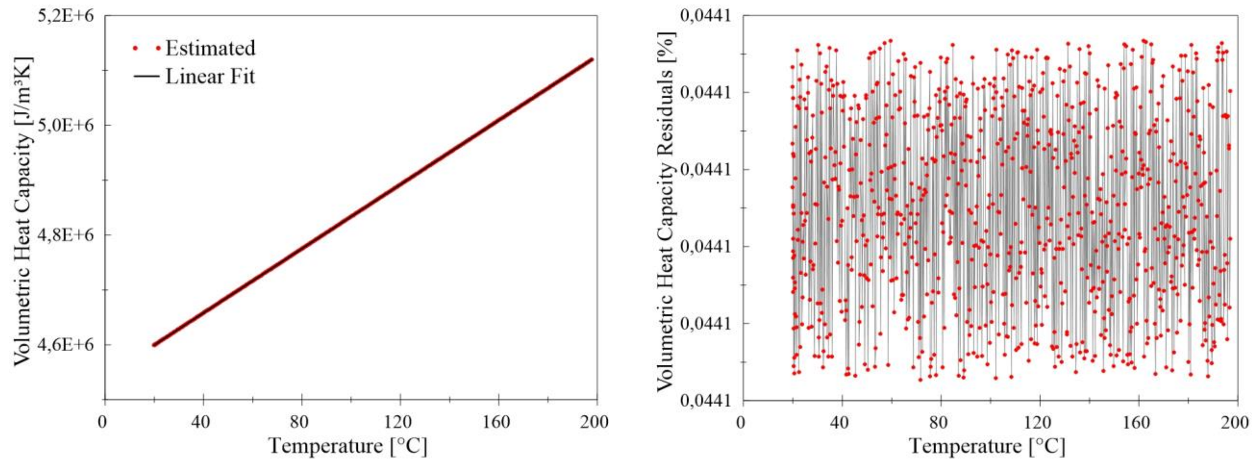
$$\rho c_p(T)=(0{,}002926\ T+4{,}34109\ )10^6\frac{\mathrm{J}}{\mathrm{m^3K}} \tag{15}$$

The curves resulting from the estimation and their linear fit are shown in Figures 4 and 5. For thermal conductivity the maximum residuals from the regression are around 0.6% of the actual value and for the volumetric heat capacity such deviations are less than 0.05%. Due to the smaller temperature sensitivity to *k*, results might be noisier and more susceptible to residuals. Although, the correlation coefficients (R-squared) resulted in 0.998 and 1 respectively, which shows the fit reliability.



(a) (b)

Figure 4. (a) Estimated thermal conductivity and (b) Residuals.



(a) (b)

Figure 5. (a) Estimated volumetric heat capacity and (b) Residuals.

Furthermore, as far as a simulated study is concerned, there must consistency between estimated and simulated values. Considering both properties varying as Eq. (16), Tab. 1 presents the comparison between the experimental curve used in the simulation and the result presented in this work.

$$P(T) = p_1 T + p_2 \quad (16)$$

Table 1. Coefficients of the experimental and estimated regression curves.

Property	Coefficient	This work	Carollo *et al.* (2019)	Difference [%]
k [W/mK]	k_1	0.01057	0.01067	0.94
	k_2	15.4364	15.4293	0.05
ρc_p [J/m³K]	ρc_{p1}	2926	2926.6	0.02
	ρc_{p2}	4341090	4343130	0.05

As previously mentioned, the thermal conductivity presents a larger variation due to the fact of the lower sensitivity. Nevertheless, as expected, the estimated values are compatible to the ones presented in the simulation. Their small difference, caused by the addition of random errors in the temperature data, confirms the accuracy of the method.

4. CONCLUSIONS

This work has presented a nonlinear inverse heat conduction problem technique to estimate simultaneously temperature-dependent thermal conductivity and volumetric heat capacity of an AISI 304 stainless steel sample. This study is important when designing processes with high temperature variation. The iterative technique based on the Gauss method of minimization has shown great efficiency in the sequential and simultaneous estimation. Although it presents high computational cost and may show instability in the calculation of gradients, both properties have shown satisfactory results. Through linear regression, curves have presented residuals around 0.6% for k and 0.05% for ρc_p, besides correlation residuals close to one. In addition, when compared to literature, deviations were less than 1% and 0.05%, respectively.

Although the use of simulated experimental data is simple and affordable in heat transfer applications, the use of experimental data in the estimation process is an objective for future work. Finally, the methodology can be applied in thermal models with different geometries and boundary conditions

5. ACKNOWLEDGEMENTS

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