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A TIME TRAVELING REGULARIZATION METHOD FOR THREE DIMENSIONAL INVERSE PROBLEMS IN HEAT CONDUCTION

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Abstract. *The Time Traveling Regularization (TTR) is a regularization methodology for the solution of inverse problems. The TTR must be applied together with an optimization technique, for this work the Golden Section was used. One of the big advantages of the use of this methodology is the noise reduction of the outputs results on inverse problems in heat conduction. In this work, a methodology is proposed for the heat flux estimation in a three-dimensional heat conduction inverse problem. The methodology was based on the Golden Section and TTR. To validate the methodology, lab-controlled experiments were performed in a AISI 304 sample. The three-dimensional direct model was solved from the finite differences method. The heat flux was estimated through the TTR and Sequential Function Specification Method (SFSM). Both methods presented similar results with low variation between the estimated heat flux. The similarity among the obtained results and the heat flux values generated by the resistive heater, as well the low temperature residues, validate the proposed methodology*.

Keywords: *Inverse Problems, Nonlinear Heat Transfer, Time Traveling Regularization, Function Specification Method, Optimization.*

1. INTRODUCTION

Due to the necessity of industrial application and science in general, the field of inverse problems has grown in the last decades. These problems can be applied in process of computer tomography, nondestructive experiments, shape optimization and geophysics problems for example. Also, the inverse heat conduction problem (IHCP) can be used to study complex manufacturing problems as welding and machining processes.

The inverse problem is an ill-posed problem, thus it does not follow at least one of the criteria established by Hadamard (1902) to classify well-posed problems. In this case, the IHCP does not follow the third criterion, which is the continuity relation between the solution and the input data. In other words, the IHCP can be considered as a cause and effect problem. In the direct problem the causes are known (boundary conditions and thermal properties) and it is desired to obtain the temperature field in the domain (the effect). However, in the inverse problem the causes are unknown and estimated by the observation of the variation of effects over time. The classical IHCP is the determination of the unknown heat flux boundary condition by monitoring the temperature data in one or more points of the domain.

The temperature data provided for the solution of the IHCP contains inherent errors caused by the measuring instruments. Thus, it is important to note that the estimated values obtained for the desired parameters are strongly affected by these errors since the problem is ill-posed. Therefore, the results obtained are estimates and the main objective is to approximate the estimated values as much as possible to the real values. Thus, besides using regularization techniques, the experimental procedure should be performed optimally in order to minimize the noise in the experimental data.

One of the pioneers in inverse heat conduction problems was Stoltz (1960), who proposed a method to determine the heat flux on the surface of spheres during a quenching process. The Stoltz method is easy to implement, but very sensitive to noise in temperature data. To minimize this problem, Beck *et al.* (1985) proposed a regularization to Stoltz method, eliminating much of the noise in the estimated heat flux values. In addition, it used multiple temperature sensors to perform the estimation of heat flux. This method is known as Sequential Function Specification Method (SFSM). The SFSM is easy to programming and fast computationally, because the method is not iterative and the temperature variation is directly calculated by the Duhamel's theorem. The method is so fast if compared to others techniques that Najafi (2015), proposed a real time solution for an IHCP with multiple unknown heat fluxes boundary conditions. However, the method is not able to solve nonlinear problems.

Alifanov (1974) used the conjugate gradient method to estimate functions in IHCP. The method is based on an optimization process with iterative regularization. This technique is able to solve linear and nonlinear problems of function or parameters estimation.

Tikhonov and Arsenin (1977) proposed a method known as Tikhonov Regularization, which uses Duhamel's theorem and a least squares optimization in addition to a linear factor that regularize the noises present in experimental temperatures. The Thikonov Regularization is an easy technique to program, however, it requires inversion of matrices, which causes a high computational cost.

The Golden Section method (Vanderplaats, 2005) is another optimization method that can be used to heat flux estimation. The method is simple and has the advantage of not requiring the calculation of derivatives. In addition, it can be used to solve nonlinear problems. However, it is necessary the use of a regularization method to show the real behavior of the estimated function.

This paper proposes an alternative methodology to solve inverse heat conduction problems. The Time Traveling Regularization (TTR) is a regularization technique that uses the Golden Section method as optimization technique. It corrects the problem of noise caused by inherent errors in temperature measurements. TTR analyzes multiple information ahead in time to estimate the heat flux at the current time.

The study of IHCP is very important to manufacturing processes. For example, the determination of the thickness of the inner lining of a steel furnace was one of the industrial problems studied by Radmonser and Wincor (1998). The wall thickness may decrease due to the process and should be monitored. As the internal temperatures of 1500 ºC prevented any type of measures, Radmonser and Wincor modeled an inverse problem and calculated the wall thickness numerically.

The IHCP also can be applied to manufacturing process problems such as welding and machining. Magalhães et al. (2016) studied the IHCP of GTA welding process of aluminum 6065 T5. The inverse problem as solved using BFGS optimization technique. In the machining process one of the most important parameters to consider is the cutting tool life. The study of the temperature field on the cutting tool surface is very important for the development of new technologies. Because temperatures are difficult to measure near the cutting zone, an inverse approach is needed. Santos *et al.* (2014) proposed a mathematical and experimental model to estimate the heat flux at the cutting tool surface. Then, the estimated heat flux was used to calculate the temperature field by the solution of the direct problem.

In many industrial processes, the real problems are nonlinear, due to large temperature variations. For example, the mentioned welding and machining processes. However, nonlinear problems are difficult to solve, thus, many authors consider the problems linear. In this paper, in addition to proposing an alternative method of IHCP solution, it is also shown a method to use the SFSM to solve nonlinear 3D inverse problems of heat flux estimation.

In this work, the validation of TTR method for heat flux estimation in 3D models was performed. Thus, an experiment was performed on a sample of stainless steel AISI 304 at the heat transfer laboratory (LabTC) of Federal University of Itajubá (UNIFEI). The results obtained with the TTR technique were compared with de heat flux values provided by the resistive heater to validate the technique.

2. METHODOLOGY

2.1 Direct model

The direct model of the heat conduction problem studied in this paper is shown in Fig. 1. A stainless steel AISI 304 flat plate is subjected to a heat flux *q(t)*. This flux is generated by a resistive heater located at the top surface of the plate and all the other surfaces are insulated to avoid heat losses to the external environment. If the material has thermal conductivity *k*, density *ρ*, specific heat at constant pressure c_p, and initial temperature T_0, the problem is modeled by Eqs. (1):

$$\frac{\partial}{\partial x}\left(k\frac{\partial T(x,y,z,t)}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T(x,y,z,t)}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T(x,y,z,t)}{\partial z}\right)=\rho c_p\frac{\partial T(x,y,z,t)}{\partial t} \tag{1.a}$$

$$-k\left.\frac{\partial T(x,y,z,t)}{\partial n}\right|_{S1}=q(t) \tag{1.b}$$

$$\left.\frac{\partial T(x,y,z,t)}{\partial n}\right|_{S2}=0 \tag{1.c}$$

$$T(x,y,z,0)=T_0 \tag{1.d}$$

where *S1* is the surface subjected to the heat flux, *S2* is the insulated surface and *n* is the outward-drawn normal unit vector to the surface.

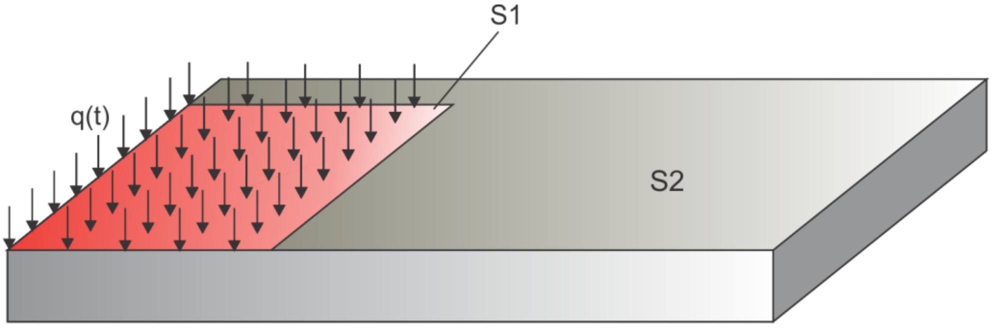

Figure 1. Stainless steel AISI 304 plate subjected to the heat flux q(t).

2.2 Sequential Function Specification Method (SFSM)

The SFSM is used to solve the inverse heat conduction problem proposed in this paper. By this method, the unknown heat flux boundary condition can be estimated.

To solve the inverse problem, is used the objective function given by Eq. (2) that minimizes the differences between the measured temperatures, Y_{M+r-1}, and the calculated temperatures, T_{M+r-1}, from time step M to r future time steps ahead.

$$S = \sum_{i=1}^{r} \left(Y_{M+i-1} - T_{M+i-1} \right)^2 \tag{2}$$

Assuming that the heat flux components $\hat{q}_1, \hat{q}_2, ..., \hat{q}_{M-1}$ are known, from time t_M to t_{M+r-1} the heat flux values are considered constants. To add stability, the future heat flux components are assumed to be equal $\hat{q}_{m-1}$, as shown in Eq. (3).

$$q_M = q_{M+1} = q_{M+2} = \ldots = q_{M+r-1} = \hat{q}_{M-1} \tag{3}$$

Using a numerical approximation of Duhamel's Theorem and the heat flux constant functional form given by Eq. (3), the temperature T_{M+i-1} can be calculated by Eq. (4),

$$T_{M+i-1} = \hat{T}_{M+i-1} + q_M \sum_{i=1}^{r} X_{M+i-1} \tag{4}$$

where $\hat{T}_{M+i-1}$ is the estimated temperature by the Duhamel's theorem and X_i are the thermal sensitivity coefficients, defined by Eq. (5):

$$X_i = \frac{\partial T_i}{\partial q_i} \tag{5}$$

Combining Eqs. (2) and (4), and optimizing the result for q_M, yields

$$q_M = \frac{\sum_{i=1}^{r} \left(Y_{M+i-1} - \hat{T}_{M+i-1} \right) X_i}{\sum_{i=1}^{r} X_i^2} \tag{6}$$

Equation (6) represents a direct formulation to estimate the heat flux step by step. It can be noted that larger is the number of future time steps, r, better is the stability of the estimated heat flux. However, if r is excessively large, the estimated heat flux curve may be super-regularized, that is, it will be very smoothed, losing the characteristics of the real heat flux curve.

The sensitivity coefficients can be calculated through the same model of the Eqs. (1). Calculating the derivatives of Eqs. (1), results:

$$k\nabla^2 X(x,y,z,t) = \rho c_p \frac{\partial X(x,y,z,t)}{\partial t} \tag{7a}$$

$$-k\frac{\partial X(x,y,z,t)}{\partial n}\bigg|_{S1} = 1 \tag{7b}$$

$$\frac{\partial T(x,y,z,t)}{\partial n}\bigg|_{S2} = 0 \tag{7c}$$

$$X(x,y,z,0) = 0 \tag{7d}$$

2.3 Time Traveling Regularization (TTR)

The technique proposed in this article consists of analyzing a hypothetical time line for each initial guess proposed by the optimization technique. Then it compares the parameter to be minimized at a future time. In other words, the method analyzes how the response of each initial guess given by the optimization method will affect the numerical temperature response at a future time. The TTR is combined with the Golden Section optimization method (Vanderplaats, 2005).

Figure 1 shows a diagram of TTR algorithm. The optimization method requires an initial guess for the variable to be minimized. From this value, the variable is considered constant from time t_{jj} to t_{jj+r}. The objective function value is compared to a small tolerance. If the guess is not enough to minimize the function, then the optimization technique will set the next value and restart de model from time step t_{jj}. The algorithm stops when the stop criterion is satisfied and advances to the next time step.

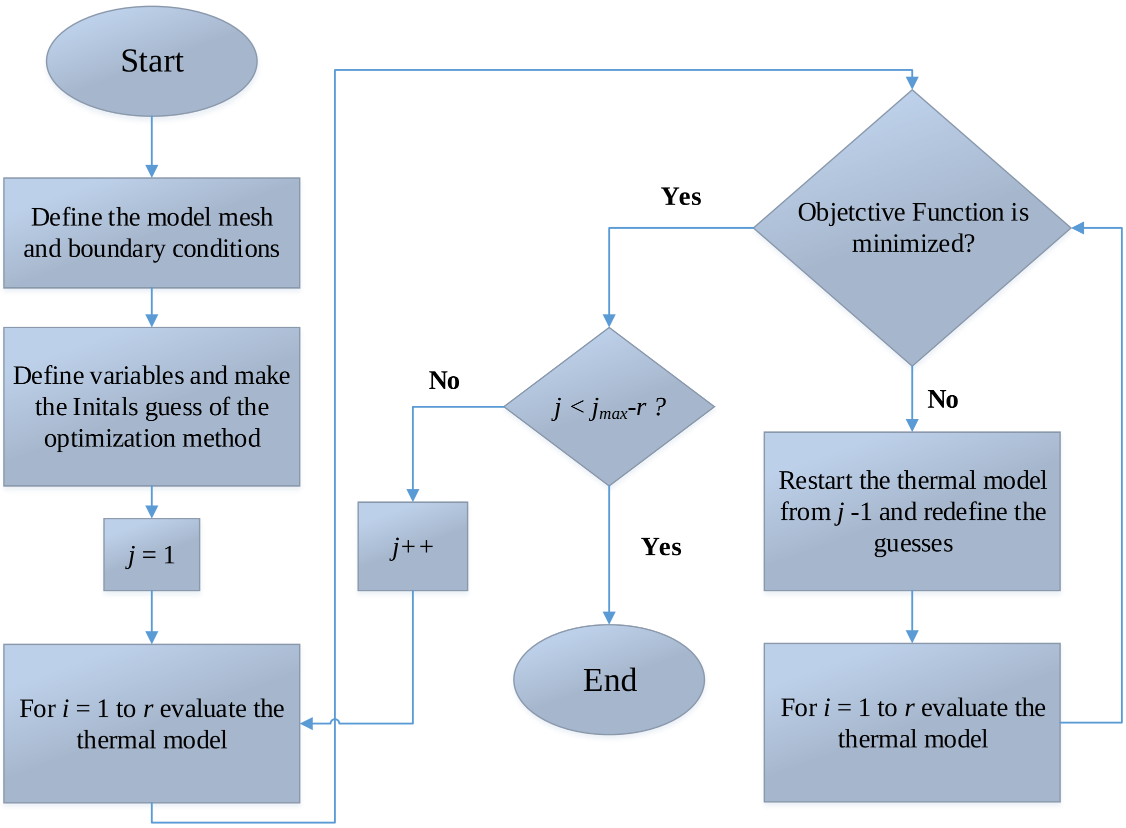

Figure 2. TTR algorithm.

The objective function to be minimized is given by Eq. (8). In this equation, the introduction of temporal analysis through TTR significantly reduces noise in the estimated parameters. When the *r* value increases, the noise decreases. Therefore, the objective function is modified to compare temperatures of several time steps ahead, resulting in Eq. (9).

$$F_{obj}^{jj} = \left(Y^{jj} - T^{jj}\right)^2 \tag{8}$$

$$F_{obj}^{jj} = \sum_{i=0}^{jj+r}\left(Y^{jj+i} - T^{jj+i}\right)^2 \tag{9}$$

2.4 Iterative Sequential Function Specification Method

In cases of nonlinear heat conduction problems, the classical SFSM approach based on the calculation of temperatures by Duhamel's theorem cannot be used. In this case, an iterative technique based on Gauss Minimization Method (Beck and Arnold, 1977) will be presented.

Let $\vec{T}$ be a vector of observations of size *n* whose formulation depends on a vector of unknown parameters β of length *p*. If β varies $\Delta\vec{b}$, then the temperature at a point of the domain can be approximated by an expansion in Taylor series, as shown in Eq. (10).

$$\vec{T}\Big|_{\vec{b}+\Delta\vec{b}} = \vec{T}\Big|_{\vec{b}} + \frac{\partial\vec{T}}{\partial\beta}\Big|_{\vec{b}}\Delta\vec{b} \tag{10}$$

The gradient in Eq. (10) is the sensitivity matrix and can be represented by Eq. (11).

$$[X_\beta] = \frac{\partial\vec{T}}{\partial\beta}\Big|_{\vec{b}} = \begin{bmatrix} \frac{\partial T_1}{\partial\beta_1} & \frac{\partial T_1}{\partial\beta_2} & & \frac{\partial T_1}{\partial\beta_p} \\ \frac{\partial T_2}{\partial\beta_1} & \frac{\partial T_2}{\partial\beta_2} & \cdots & \frac{\partial T_2}{\partial\beta_p} \\ \vdots & & \ddots & \vdots \\ \frac{\partial T_n}{\partial\beta_1} & \frac{\partial T_n}{\partial\beta_2} & \cdots & \frac{\partial T_n}{\partial\beta_p} \end{bmatrix} \tag{11}$$

To solve the inverse problems the objective function given by Eq. (12) must be minimized.

$$S = \left(\vec{Y} - \vec{T}\right)^T\left(\vec{Y} - \vec{T}\right) \tag{12}$$

Substituting Eqs. (10) and (11) in Eq. (12), and minimizing it for {b}, results:

$$\Delta\vec{b} = \left([X_\beta]^T[X_\beta]\right)^{-1}[X_\beta]^T\left(\vec{Y} - \vec{T}\Big|_{\vec{b}}\right) \tag{13}$$

Note that in the IHCP studied in this work, the parameter β has only one component, which is the heat flux *q(t)*, thus $\Delta\vec{b} = \Delta q$. For each time step *M*, the increment of heat flux Δq must be computed until the Eq. (14) reaches convergence.

$$q_M^{(i+1)} = q_M^{(i)} + \Delta q_M^{(i)} \tag{14}$$

3. EXPERIMENTAL PROCEDURE

In order to validate the methodology proposed in this paper, it was performed a three-dimensional heat conduction experiment on AISI 304 stainless steel samples at Heat Transfer Laboratory of Federal University of Itajubá.

Figure 3 represents AISI 304 sample dimensions used in the experiment. The dimensions of the resistive heater, used to provide the heat flux on the top surface, are shown in Fig. 4. It is observed that the three-dimensional behavior is guaranteed, since the heat flux is restricted in a small area of the top surface.

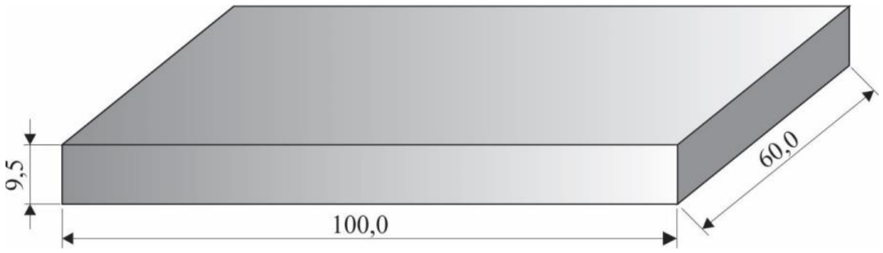

Figure 3. AISI 304 sample dimensions.

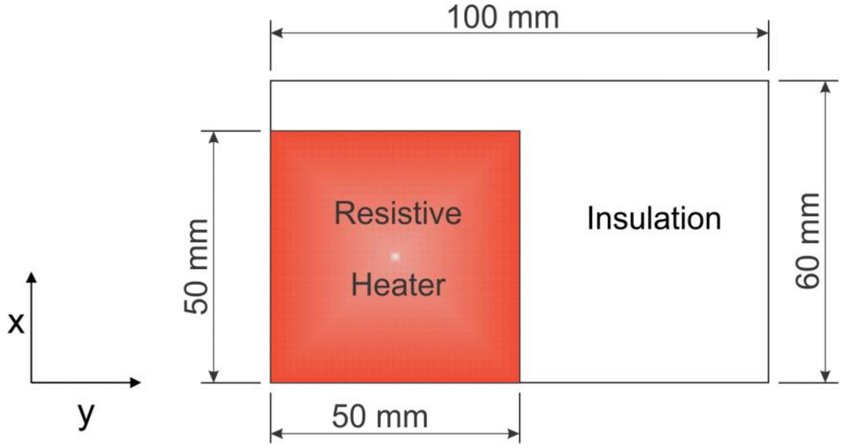

Figure 4. Resistive heater dimensions.

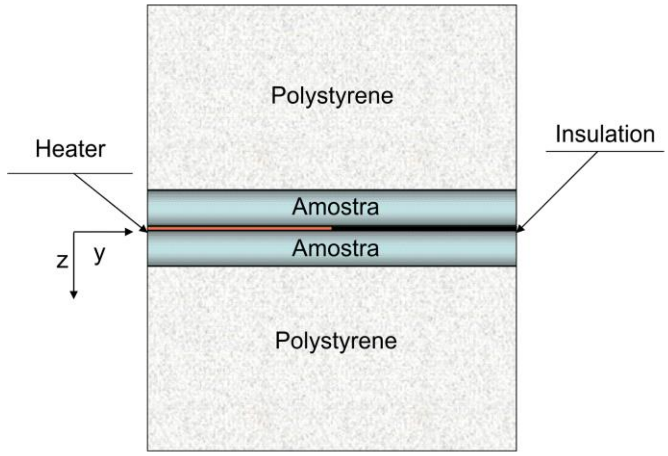

Figure 5. Symmetrical assembly of the experiment.

The experimental assembly is shown in Fig. 5. It is important to mention that all the surfaces of the samples were insulated. The experiment carried out has symmetrical assembly to ensure that all heat flux is transmitted to the samples, avoiding losses.

To provide the necessary heat flux, a kapton resistive heater with resistance of 15 Ω was used. The advantage of using this type of heater is due to its small thickness and good malleability. In order to minimize the contact resistance between heater and sample, the silver thermal paste Arctic Silver 5 was used. The heater is connected to the Instrutemp ST 305-II power supply. To measure the experimental temperatures, the Cormel/Alumel – 30 AWG thermocouple, welded by capacitive discharge, was used. The thermocouple was located at the coordinate $(x,y,z)=(25.0,25.0,9.5)$ mm on the base of the sample and at the center of the resistive heater.

4. RESULTS

To calculate the temperature distribution of the three-dimensional direct problem, a computer program was developed using the finite element method with Galerkin methodology. A tetrahedral mesh was generated with 20078 elements. The thermophysical properties considered for AISI 304 were obtained from Carollo (2010), with thermal conductivity 14.61 W/mºC and thermal diffusivity of 3.74 x 10^{-6} m^2/s. The sample was initially at 19.5 ºC. The experiment lasted 240 s, and at first the heater was kept off for 40 s, then switched on at an average power of 2000 W/m^2 to the time of 200 s and turned off again. Figure (6) shows the experimental data measured by the thermocouple.

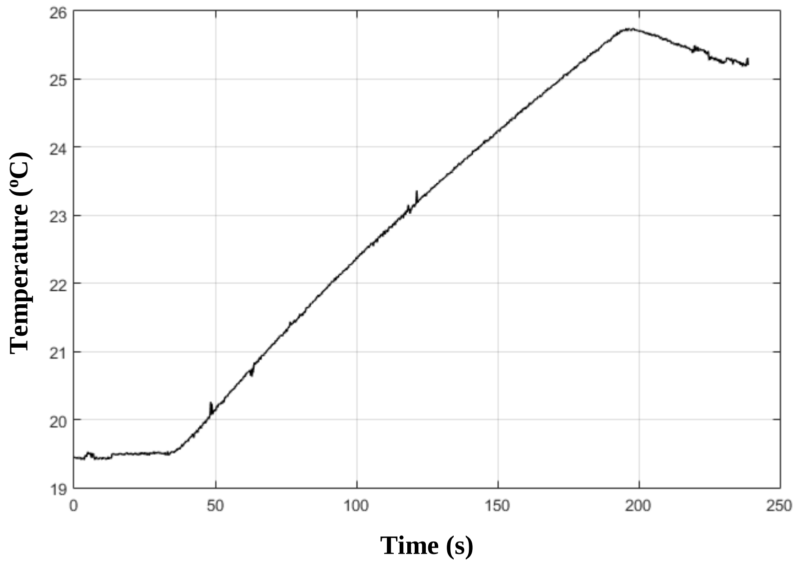

Figure 6. Measured temperature data.

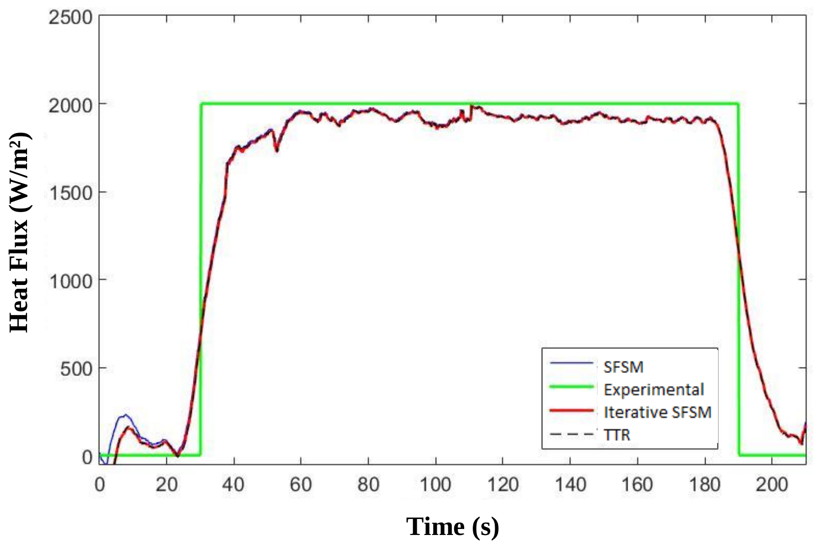

Figure 7. Comparison between heat flux estimated by TTR, Function Specification Method and the theoretical flux provided by the heater.

The heat flux was estimated by TTR and SFSM and iterative SFSM using 55 future time steps to each one. Figure 7 shows the results obtained for heat flux estimation comparing with its theoretical value. It is observed that heat flux behavior estimated by the three techniques is the same and represents well the thermal input generated by the resistive heater. Note that the estimated heat flux values are slightly below the experimental curve. This can be explained by the fact that electrical resistance, due to the length of the heater wires, were not considered.

Figure 8 shows the residuals between the heat fluxes estimated by the techniques and the experimental flux. It can be observed that the residuals are very low compared to the value of 2000 W/m² of the real heat flux. In the region where the heater reaches stability, the mean residue between the experimental heat flux and the estimated is 95 W/m² and the standard deviation of 43 W/m².

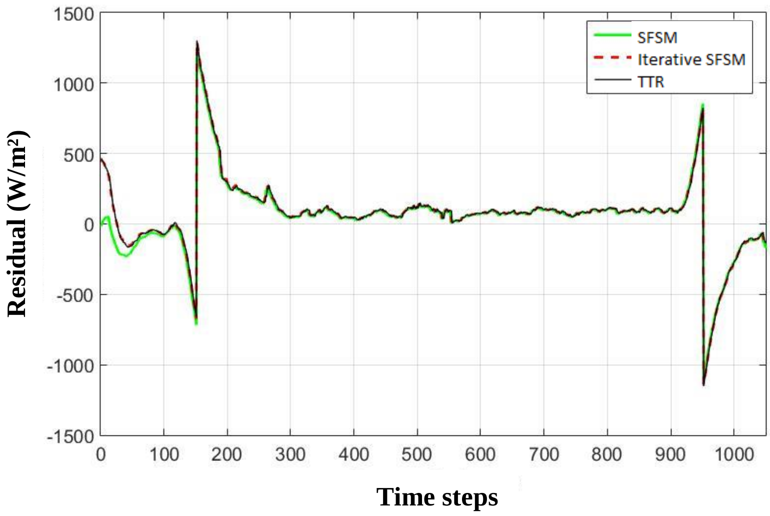

Figure 8. Residuals

Figure 9 shows the residual values between the heat flux estimated by TTR and SFSM. It is observed that the residuals are very low compared to the value of the heat flux (2000 W/m²). In the region of interest, where the heater reaches the steady state, the difference between the two techniques is minimal, obtaining an average value of 1.63 W/m² with a standard deviation of 6.34 W/m².

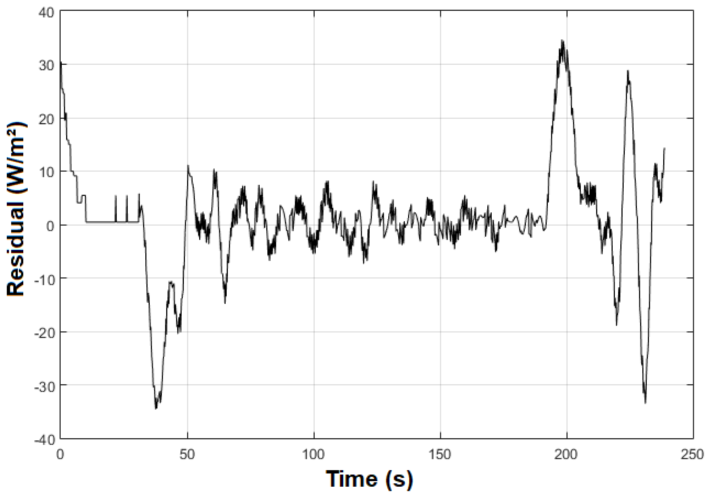

Figure 9. Residuals between the heat flux values estimated by TTR and SFSM.

Figure 10 shows the comparison between the temperatures calculated by the estimated heat fluxes and those measured by the thermocouple. The temperatures values obtained by the direct problem are very close to the experimental ones, with larger differences in regions of greater derivative. The residuals between the estimated and experimental temperatures are shown in Figure 11. The temperatures calculated by the SFSM presented larger errors if compared to the other methods, with mean residue of 0.063 ºC and deviation of 0.026 ºC. Otherwise, the iterative SFSM had the lowest residue values with mean of 0.002 ºC and deviation of 0.022 ºC. The TTR method also presented low residual values with mean of 0.011 ºC and deviation of 0.025 ºC.

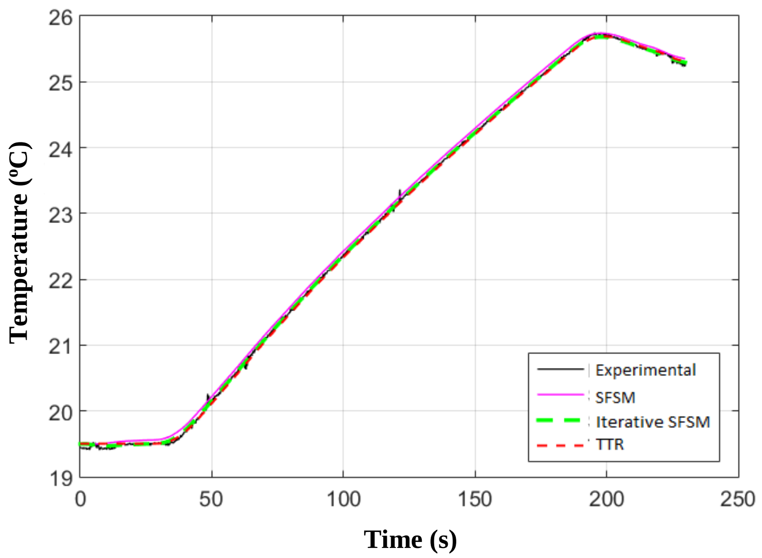

Figure 10. Experimental and estimated temperatures.

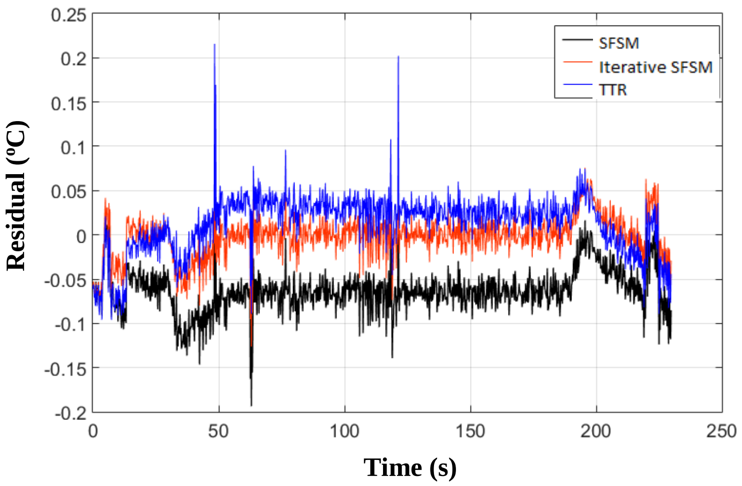

Figure 11. Residuals between experimental and estimated temperatures.

5. CONCLUSIONS

This work presents a comparison between three techniques used to estimate the heat flux of inverse heat conduction problems. In order to obtain good comparative results, experiments were performed on stainless steel AISI 304 with the heat flux defined by a step function. The experimental temperatures measured at one point on the sample was used to estimate the heat flux by the method proposed in this paper (Golden Section with TTR), the SFSM proposed by Beck *et al.* (1985) and the iterative SFSM. The estimated heat flux values were compared with the experimental heat flux provided by the resistive heater, showing very precisely results. Since the SFSM is an established method in literature, it can be concluded that the heat flux estimation by TTR is reliable to estimate heat flux boundary conditions.

The TTR methodology has the advantage of not requiring the calculation of numerical derivatives, as opposed to the SFSM, that requires the evaluation of the thermal sensitivity coefficients. The iterative techniques (TTR and iterative SFSM) showed better results. In addition, they can be used for nonlinear problems. However, the classical has the lower computational time.

6. ACKNOWLEDGEMENTS

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