18th Brazilian Congress of Thermal Sciences and Engineering
November 16-20, 2020 (Online)

ENC-2020-0081
ANALYSIS OF LINEAR AND NONLINEAR INVERSE PROBLEM TECHNIQUES FOR SOLVING A THREE-DIMENSIONAL HEAT CONDUCTION PROBLEM

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Abstract. *Inverse Heat Conduction Problems are those in which an unknown parameter in the heat diffusion equation needs to be estimated using measured temperature data. The possible approaches for those problems become even more difficult when those measured temperatures vary widely, turning the problem non-linear. In this work, a comparison between two techniques for the heat flux estimation in a three-dimensional heat conduction inverse problem is performed. To solve the direct problem the three-dimensional heat diffusion equation is discretized by the Finite Difference method. The inverse problem is solved first using the linear Sequential Function Specification Method and secondly the iterative non-linear Sequential Function Specification Method. The validation of the methods is done through a non-linear simulation with a Tungsten Carbide sample and an experiment with an AISI 304 stainless steel sample. The estimated heat fluxes are showed and compared each other, being also compared with the simulated and the real ones.*

Keywords: *Inverse Problems, Nonlinear Heat Transfer, Optimization, Sequential Function Specification Method*

1. INTRODUCTION

The necessity of understanding and controlling the physical, chemical and biological phenomena made the engineering and scientists study the inverse problems. Talking specifically on heat transfer, the estimation of unknown heat fluxes is considered an inverse problem, so called Inverse Heat Conduction Problem (IHCP). As the improvement and understanding of crucial engineering process, such as quenching, welding and machining, requires this heat flux estimation, several methods were developed trying to achieve this goal.

As in other fields, in the heat conduction there is the distinction between the direct and the inverse problems. The direct is the one that calculates the temperature field in a body, solving the heat diffusion equation with information of initial and boundary conditions, thermal properties and geometry. This problem has a cause and effect relationship, being relatively simple to solve.

Otherwise, the inverse problem is not simple. The classical IHCP is the estimation of a missed boundary condition, the heat flux, using the temperature historical in one or more points of the heated body. The complexity of inverse problems arises in their ill-posedness. Based on Hadamard (1902) well-posed problems follow the criteria of existence, uniqueness and stability of solution, while the ill-posed fail in at least one of these criteria.

The IHCP normally fails to ensure the stability of the solution, in other words, small changes in the input can result in huge changes in the output. This characteristic becomes very concerning as in the IHCP the temperature historical data used to solve the problem is collected by thermocouple measurements, what inherently brings errors, that can change significantly the estimated heat fluxes.

Due to this problem of stability, the IHCP usually uses not only an optimization technique, that minimizes the sum of the squares of the errors between the estimated and the measured temperatures with respect to the unknown heat fluxes. But also, needs a regularization method, that reduces the instability of the solution and makes the heat flux curve smoother, thus more similar to the expected real curve format.

One of the most important studies in the inverse heat conduction problems was done by Stolz (1960). In order to estimate the surface heat flux on spheres over a quenching process, he developed a method known as “exact matching”. In this method, during the estimation of an instantaneous heat flux, the estimated temperature is made exact to the measured one. The estimation process is sequential (calculating the heat flux value at each step in time) and not interactive, using the Duhamel’s theorem to calculate the temperature variation. Although the huge importance of this method, as being a pioneer, it is problematic, very sensitive to measurement errors and to small steps in time. The main cause of these problems is the lack of a regularization method. With the aim of solving this, Beck et al. (1985), developed a new method, based on the Stolz Algorithm, the Sequential Function Specification Method (SFSM). The SFSM uses not only the information of temperature at the same moment of the desired heat flux, but also information of future temperatures, so regularizing the solution, decreasing the instability, and allowing the usage of small steps in time.

A method of regularization was proposed by Tikhonov and Arsenin (1977). Known as Tikhonov Regularization, the technique also uses Duhamel's and a least squares minimization, employing a linear factor that regularizes the noise inherent to the experimental temperatures.

Based on Tikhonov Regularization, Najafi et al. (2015) developed a real time solution for IHCP in a two-dimensional plate with multiple heat fluxes at the surface. The presented method uses the digital filter form of Tikhonov Regularization with data from several temperature sensors to estimate the multiple unknown heat fluxes. It is shown that near real-time heat flux estimation is possible, using just a few number of previous and future time steps with temperature information. However, to achieve good accuracy, it is necessary to have an idea about the heat flux curve's shape.

Another regularization methodology was proposed by Magalhães et al. (2018), the Time Traveling Regularization (TTR). This technique, which was used together with the Golden Section optimization method, modifies the objective function in order to have a temporal analysis during the optimization process, so regularizing the solution. The TTR with the Golden Section presented good results when compared to the SFSM, furthermore, the technique ability to handle with non-linear problems is highlighted.

Najafi and Woodbury (2015) proposed an online heat flux estimation using Artificial Neural Network (ANN) as a digital filter approach. The method uses ANN similarly as a filter based technique, training and performing the network with several previous and future temperature data to estimate the current heat flux value. The study showed good results, for both linear and non-linear cases, using a few number of these previous and future temperature data, especially when the network was trained and tested in a similar pattern and in heating, not cooling, process.

As in a great number of the engineering processes, like quenching, machining and welding, the materials are submitted to a large temperature variation, characterizing these processes as being non-linear, this paper aim is to compare the Sequential Function Specification Method, both the linear and the non-linear, for solving non-linear problems. To make the comparison, a simulated and an experimental process were carried out, in the first case simulating a heating in a Tungsten Carbide sample and, in the second, heating a AISI 304 sample. The samples were heated on part of one surface and insulated on the others; the temperature information was collected on an insulated surface of each sample. In the two cases, the heat flux histories were estimated for both methods and then compared. After it the results were showed and discussed.

2. METHODOLOGY

2.1 Direct Model

The direct model used in the IHCP is based in the Fig. 1.

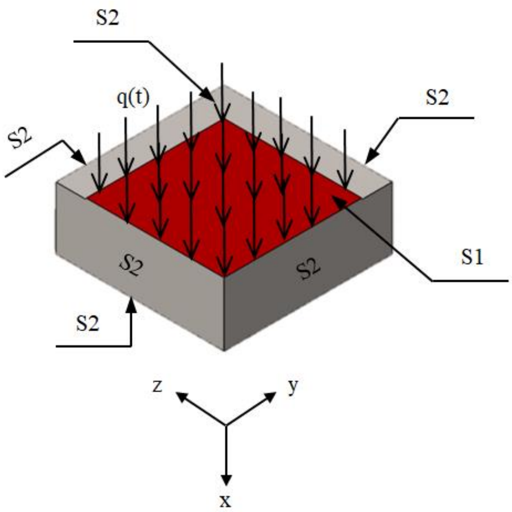

Figure 1. Transient 3D heat conduction problem.

In Figure 1 is possible to see one surface of the plate partially suffering the action of the heat flux, $q(t)$, while the other surfaces are isolated, avoiding heat losses. The mathematical description of this problem is expressed by the heat diffusion equation:

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

$$\text{in } 0 \le x \le L;\ 0 \le y \le H;\ \ 0 \le z \le W;\ \ 0 \le t \le t_f \tag{1b}$$

in which T is the temperature, $k(T)$, $\rho(T)$ and $c_p(T)$ are, respectively, the thermal conductivity, the density and the specific heat of the material, all temperature-dependent. L, H and W are the sample respective dimensions in the Cartesian Coordinates x, y and z, t is the physical time and t_f the total duration of the experiment or simulation.

Furthermore, the complete mathematical description of the problem needs the boundary and initial conditions:

$$-k(T)\frac{\partial T(x,y,z,t)}{\partial x}\bigg|_{S1} = q(t) \tag{2a}$$

$$\frac{\partial T(x,y,z,t)}{\partial n}\bigg|_{S2} = 0 \tag{2b}$$

$$T(x,y,z,t = 0) = T_0 \tag{2c}$$

in which T_0 is the initial temperature, S_1 is the surface exposed to the heat flux, S_2 is the insulated and n is the unit vector normal to the surface.

This direct problem, modeled by the heat diffusion equation with the boundary and initial conditions, is solved using the implicit Finite Difference method, as it allows working without restrictions in the size of the time steps and mesh refinement, being unconditionally stable.

2.2 Sequential Function Specification (SFSM)

The classical SFSM is the first method used to solve the IHCP in this paper. This method sequentially estimates the heat flux, step by step in time. During the heat flux estimation in a current time, it is assumed that the previous heat fluxes are known and some future heat fluxes are used, to regularize the solution, being considered in a functional form. In this work the assumed form is the constant function.

In the development of the SFSM the local temperature in a sample for a time t_M and using r future times can be determined as:

$$\boldsymbol{T} = \boldsymbol{Xq} + \widehat{\boldsymbol{T}}\Big|_{q=0} \tag{3}$$

in which $\boldsymbol{T}$ is the vector of real temperatures:

$$\boldsymbol{T} = \begin{bmatrix} T_M \\ T_{M+1} \\ \cdots \\ T_{M+r-1} \end{bmatrix} \tag{4}$$

$\boldsymbol{q}$ is the vector of heat fluxes:

$$\boldsymbol{q} = \begin{bmatrix} q_M \\ q_{M+1} \\ \cdots \\ q_{M+r-1} \end{bmatrix} \tag{5}$$

$\boldsymbol{X}$ is the matrix of thermal sensitivity coefficients:

$$\boldsymbol{X} = \begin{bmatrix} \Delta\varnothing_0 & & & \\ \Delta\varnothing_1 & \Delta\varnothing_0 & & \\ \vdots & \vdots & & \\ \Delta\varnothing_{r-1} & \Delta\varnothing_{r-2} & \cdots & \Delta\varnothing_0 \end{bmatrix} \tag{6}$$

$\widehat{\boldsymbol{T}}$ is the vector that owns the temperatures calculated by the thermal model until the time t_M, using the before estimated heat fluxes $\hat{q}_1, \hat{q}_2, \cdots, \hat{q}_{M-1}$, but with q_M considered equal to zero:

$$\hat{\boldsymbol{T}}\Big|_{q=0} = \begin{bmatrix} \sum_{i=1}^{M-1} \hat{q}_i \Delta\emptyset_{M-i} + T_0 \\ \sum_{i=1}^{M-1} \hat{q}_i \Delta\emptyset_{M-i+1} + T_0 \\ \vdots \\ \sum_{i=1}^{M-1} \hat{q}_i \Delta\emptyset_{M-i+r-1} + T_0 \end{bmatrix} \tag{7}$$

and being the components of the sensibility matrix, $\Delta\emptyset_i$:

$$\Delta\emptyset_0 = \emptyset_1 - \emptyset_0,\ \Delta\emptyset_1 = \emptyset_2 - \emptyset_1,\ \cdots,\ \Delta\emptyset_i = \emptyset_{i+1} - \emptyset_i \tag{8}$$

where $\emptyset_i$ is the temperature gain in the thermocouple position for a unitary heat flux. The sensitivity matrix components can be calculated, according to Beck and Woodbury (2016), using the temperature responses from the proposed thermal model applying a unitary heat flux.

The temporary assumed constant form of the future heat fluxes reduces the components of q to a unique value, as:

$$q_M = q_{M+1} = q_{M+2} = \cdots = q_{M+r-1} \tag{9}$$

this reduction turns the equation system stable and overdetermined.

The objective function, S, is mathematically determined as:

$$S = \sum_{i=1}^{r} \left(Y_{M+i-1} - \hat{T}_{M+i-1}\Big|_{q=0} - \emptyset_i q_M \right)^2 \tag{10}$$

where Y_M is the measured temperature at a M step in time.

This function is minimized with respect to q_M, then giving the equation that estimates this unknown:

$$\hat{q}_M = \frac{\sum_{i=1}^{r} \left(Y_{M+i-1} - \hat{T}_{M+i-1}\Big|_{q_M = \dots = 0} \right) \emptyset_i}{\sum_{i=1}^{r} \emptyset_i^2} \tag{11}$$

2.3 Iterative Sequential Function Specification Method

When the heat conduction problem is treated as nonlinear, the classical SFSM cannot be used because of its roots in the Duhamel theorem. In this case, the iterative SFSM, which is based on the Gauss Minimization Method (Beck and Arnold, 1977), is used.

Considering $\boldsymbol{T}$ a vector of observations of a length *no* which is depend on a vector of unknown parameters $\boldsymbol{\beta}$ of a length *np*, if a variation of $\Delta\boldsymbol{b}$ is applied to this vector, so the temperature at a given point of the domain can be approximated though the truncated Taylor's series:

$$\boldsymbol{T}\big|_{\boldsymbol{b}+\Delta\boldsymbol{b}} \approx \boldsymbol{T}\big|_{\boldsymbol{b}} + \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{\beta}}\Big|_{\boldsymbol{b}} \Delta\boldsymbol{b} \tag{12}$$

The gradient in Eq. (15) is the $n \times p$ matrix of sensitivity coefficients:

$$\boldsymbol{X_\beta} = \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{\beta}} = \begin{bmatrix} \frac{\partial T_1}{\partial \beta_1} & \frac{\partial T_1}{\partial \beta_2} & \cdots & \frac{\partial T_1}{\partial \beta_{np}} \\ \frac{\partial T_2}{\partial \beta_1} & \frac{\partial T_2}{\partial \beta_2} & \cdots & \frac{\partial T_2}{\partial \beta_{np}} \\ \vdots & \vdots & \ddots & \\ \frac{\partial T_{no}}{\partial \beta_1} & \frac{\partial T_{no}}{\partial \beta_2} & \cdots & \frac{\partial T_{no}}{\partial \beta_{np}} \end{bmatrix} \tag{13}$$

In order to solve the inverse problem, an objective function, S, is used:

$$\boldsymbol{S} = (\boldsymbol{Y} - \boldsymbol{T})^T - (\boldsymbol{Y} - \boldsymbol{T}) \tag{14}$$

Substituting Eqs. (12) and (13) in Eq. (14) and minimizing it for $\Delta\boldsymbol{b}$**,** results:

$$\Delta\boldsymbol{b} = \left(\boldsymbol{X_\beta^T X_\beta}\right)^{-1} \boldsymbol{X_\beta^T}(\boldsymbol{Y} - \boldsymbol{T}|_{\boldsymbol{b}}) \tag{15}$$

In the IHCP studied in this work the parameter $\boldsymbol{\beta}$ has only one component, that is the heat flux, $\boldsymbol{q}(t)$, thus $\boldsymbol{\Delta b} = \boldsymbol{\Delta q}$. For the estimation of the heat flux at each step time M the increment Δq must be computed until Eq. (16) reaches convergence.

$$\boldsymbol{q}^{(i+1)} = \boldsymbol{q}^{(i)} + \Delta\boldsymbol{q}^{(i)} \tag{16}$$

3. EXPERIMENTAL PROCEDURE

In order to validate the proposed method, first, a three-dimensional simulation considering a Tungsten Carbide sample was done. Moreover, to reinforce the methods' validation, a one-dimensional experiment using a AISI 304 sample was carried out. The fact of the experiment being considered one-dimensional is not a restriction, as the three-dimensional approach in the methodology is also suited to solve that type of problem.

3.1 Simulation using Tungsten Carbide

The simulation considered a Tungsten Carbide sample with 12.7 × 12.7 × 4.7 mm^3 dimensions. A 10.4 × 10.4 mm^2 resistive heater was positioned in the superior surface of the plate, generating a heat flux mathematically represented by the following equation:

$$q(t) = -3.2t^2 + 800 \tag{17a}$$

$$0 < t < 250 \tag{17b}$$

Both the sample and the resistive heater can be visualized in the Fig. 2.

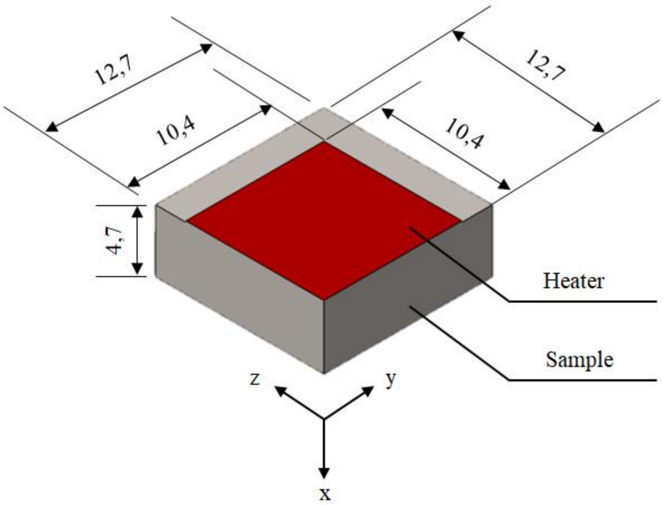

Figure 2. Tungsten Carbide sample and resistive heat dimensions.

In a real experiment, a thermocouple located at some point of the sample is necessary, as this equipment provides the temperature data to solve the ICHP. Thus, in a simulation, some point of the sample needs to be chosen, as if at it had a thermocouple, so providing the temperature records at that point. In this simulation, the chosen point was the one at the 4.7 mm; 3.5 mm; 9.5 mm coordinates.

The temperature data at his point was generated by applying the simulated heat flux in the direct model, which is numerically approximated by the Finite Difference method. Moreover, the temperature record in an experiment is expected to be carried with some errors, mainly related with electrical noisy and thermocouple's uncertainties. To simulate it, random normally distributed errors between -0.5; 0.5 °C were added to the generated temperature history.

The simulation lasted 250 s, with 0.2 s of time steps, totalizing 1251 temperature points collected. From Grzesik et al. (2009) both the constants and temperature-dependent thermal properties were obtained. The thermal conductivity assumed for the Tungsten Carbide to be used in the classical SFSM was 33.7 W/m.K, while the thermal diffusivity, α, was 3.88×10^{-5} m²/s. For the iterative SFSM the temperature-dependent thermal properties were approximated by finding functions that best fit the properties' curves found from the authors:

$$k(T) = 2.132\times10^{-9}T^3 - 1.086\times10^{-5}T^2 + 0.02121T + 33.07 \tag{18a}$$

$$\alpha(T) = \frac{-4.674\times10^{-9}T^2 + 2.092\times10^{-5}T + 0.0006484}{2.77 + T} \tag{18b}$$

Being important to emphasize that the process to find the thermal properties for the Tungsten Carbide is especially difficult as it has a large variety of possible compositions. Furthermore, it was considered that all surfaces, except the one under the heat flux action, were insulated. This simulated assembly can be visualized in the Fig. 3.

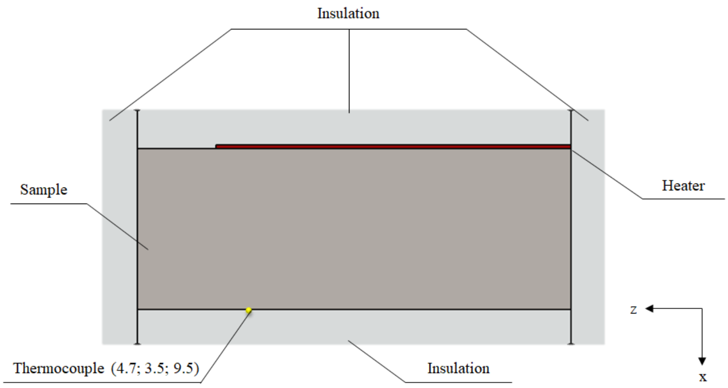

Figure 3. Simulated experiment assembly.

3.2 Experiment using AISI 304 stainless steel

In the experiment, an AISI 304 stainless steel sample with 10 mm x 50 mm x 50 mm dimensions was uniformly heated by a 50 mm x 50 mm resistive heater applied on the upper surface, while the others remained insulated. A thermocouple was positioned centrally at the surface opposite to the heated one. Due to the experiment characteristics it was considered one-dimensional, being the thermal model presented by Fig. 4.

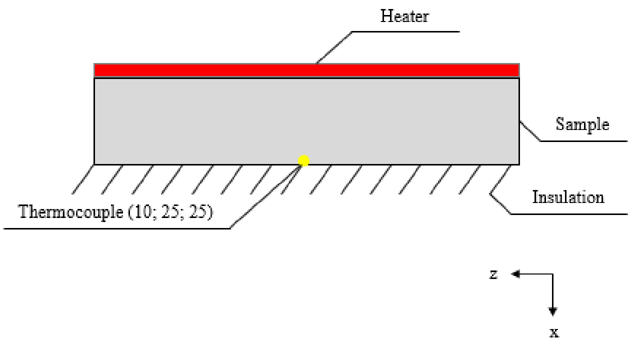

Figure 4. Experiment's thermal model.

The experiment lasted 380 s, with 0.1 s of time steps, totalizing 3801 points collected. During the first 20 s the heater was off, after it being turned on for 300 s. The thermophysical properties were obtained from Carollo (2016). For the classical SFSM, the constant temperature properties were 15.64 W/m.K for the thermal conductivity and 3.55×10^{-6} m²/s for the thermal diffusivity. For the iterative SFSM, the thermal-dependent properties obtained from the author were:

$$k(T) = 0.01067\,T + 15.4293 \tag{19a}$$

$$\alpha(T) = \frac{0.01067T + 15.4293}{(0.0029266T + 4.34313)\times10^{6}} \tag{19b}$$

4. RESULTS

4.1 Tugsten Carbide

After generating the simulated experiment, the temperature data was used for the heat flux estimation in both classical and iterative SFSM. To regularize the output 15 future time steps were used. Figure 5 compares these two estimations with the generated heat flux.

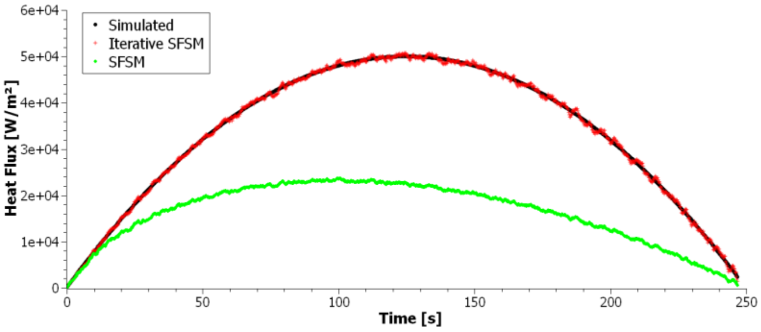

Figure 5. Comparison between simulated and estimated heat fluxes

As it may be seen, the heat flux curve calculated by the iterative SFSM is very similar to the simulated one, while the classical SFSM failed to achieve good results. The heat flux estimated by the iterative process presented average differences of approximately 1.85% compared to the simulated heat flux, whilst the estimated using the classical process produced 49,09% average differences.

In order to verify the heat fluxes effects in the temperature field, they were applied in the direct model and the temperature data at the thermocouple location was collected. In Fig. 6 it is possible to visualize the differences between these temperatures found using the estimated heat fluxes and the simulated.

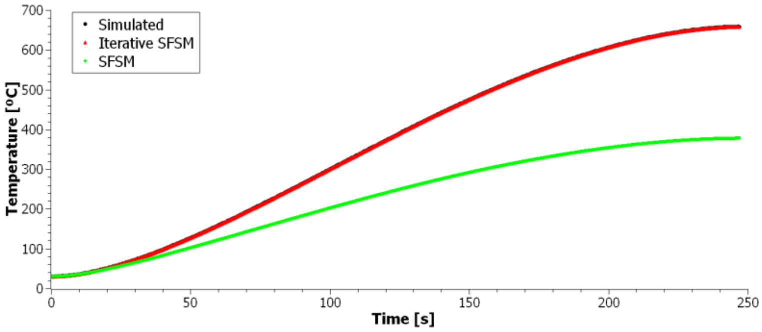

Figure 6. Temperature responses to the heat fluxes

Once more it is possible to see good results in the iterative SFSM, in which the calculated temperatures were very close to the temperature information from the simulated experiment. Moreover, the inability of the classical SFSM to solve nonlinear, problems is highlighted.

4.2 AISI 304

Similarly to the simulation, the temperature data collected by the thermocouple in the experiment was used to the heat flux estimation in both classical and iterative SFSM. The heat flux regularization was done by using 60 future time steps. In order to compare the results of the methods with the experimental heat flux, Fig. 7 is shown.

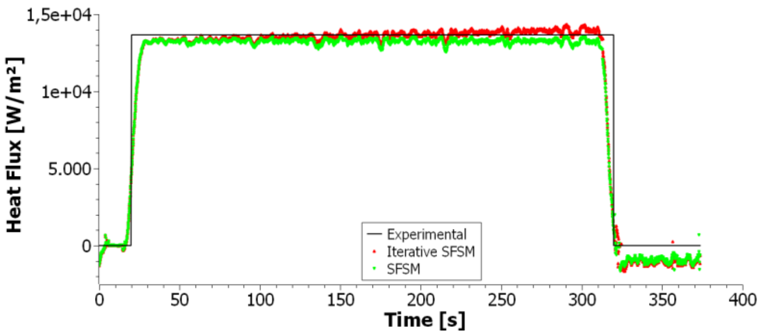

Figure 7. Estimated heat fluxes for the AISI 304 experiment.

As the experiment has reached temperatures slightly above 100 °C, that do not produce high properties variations, both methods presented small result differences. However, afresh, the iterative one produced smaller average differences than the classical SFSM. In the interval in which the heater reached stability, while the heat flux estimated by the iterative method had an average deviation of 1.60% compared to the experimental one, the heat flux estimated by the classical SFSM had an average deviation of 3.11%.

To verify the influence of these estimated heat fluxes through the sample, in terms of temperature, they were applied in the direct model. Then, the temperature at the thermocouple location was collected and compared, as shown in the Fig. 8.

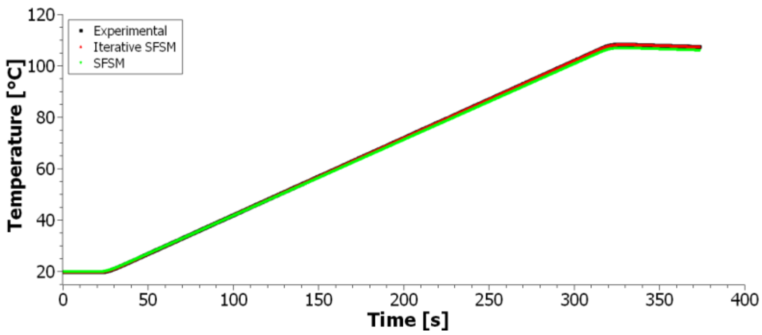

Figure 8. Comparison between the experimental temperatures and those generated by the techniques.

This figure attests the good methods' performance when they are used in inverse heat conduction problems with small temperature variation. Although the temperature's residuals between both methods and the experimental temperature data are shown in the Fig. 9, demonstrating again the better accuracy of the iterative SFSM.

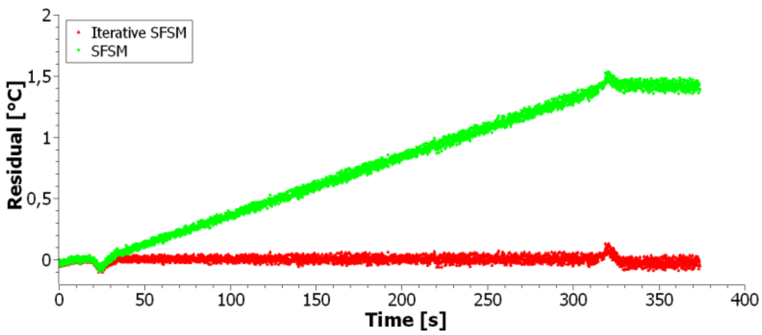

Figure 9. Temperature residuals for both methods.

From the figure, it is clear that the higher the temperature's variation, the smaller the linear method's accuracy. Thus, the importance of the use of the iterative SFSM to solve non-linear inverse heat conduction problems, as welding and machining for example, is once more highlighted.

5. CONCLUSIONS

This work presented a comparison between two techniques, the Sequential Function Specification Method and the Iterative SFSM, when used to estimate heat fluxes in non-linear inverse heat conduction problems. In order to validate the methods and better compare them, a simulation and an experiment were done. In both approaches the iterative technique produced more accurate results, especially in high temperatures' regions.

These results were expected, as the classical SFSM assumes the thermal properties as constants, without varying according to the temperature, whilst the iterative one assumes the thermal properties as temperature's dependents.

6. ACKNOWLEDGEMENTS

The authors would like to thank CNPq, CAPES and FAPEMIG for their financial support.

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