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THERMAL PROPERTIES ESTIMATION OF METALS USING DIFFERENT THERMAL MODELS

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Abstract. *This work presents two models for the simultaneous estimation of thermal conductivity, λ , and volumetric heat capacity, ρc_p , in a sample of AISI 304 stainless steel. The thermal models used are based on a transient one-dimensional heat diffusion equation. Based on the analysis of the sensitivity coefficients, two different intensities of heat flux are used on the top surface. On the bottom surface, each model has a different condition: the first one has an insulation condition and the other one has a constant temperature condition. To estimate these properties, an error function is minimized by applying the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. The numerical temperature is obtained by the solution of proposed thermal model using the Finite Difference Method with an implicit formulation. The simulated experimental temperature is obtained by the addition of residual in the numerical data. For both models, the estimated properties are in agreement with literature and presented differences around 9 %.*

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

1. INTRODUCTION

With the development of more accurate methodologies, a correct and effective knowledge of the temperature of a certain material is indispensable. Thus, knowing the temperature it can be made simulations of intense use of the material analyzed, reducing the probability of any problem during its usual condition of use. It is also possible to solve more quickly and efficiently any abnormal behavior of the material.

In engineering there is a constant search for development of materials that have better thermal properties and lower cost than materials that are already in use. Therefore, it is extremely important the existence of works such as the one presented in this article, in order to concisely determine the thermal properties and to collaborate in a significant way for the development of more efficient methods in the field of heat transfer as well as in mechanical engineering as a whole. For example, in the automotive sector we can mention the braking system, where is essential to know the temperature that the brake disc will reach. Therefore, studies must be carried out to avoid accidents, in others words, it is necessary to design a material that supports the maximum temperature during the stopping of the vehicle using a factor of safety. It is also possible to verify if there is a more appropriate material (lower price with equivalent mechanical characteristics) to compose the braking system, thus giving the manufacturer a reduction in the price of the material without losing quality.

Thereby, every engineer should be aware of the characteristics and behavior of the materials used in their projects. Knowing the properties of materials is fundamental to the project execution and control, avoiding failures, reducing costs and increasing their application.

The important thermal properties studied in this paper are: the thermal conductivity, λ , and the volumetric heat capacity, ρc_p . The thermal conductivity corresponds to the amount of heat that is transmitted across the surface of a material of constant thickness by the temperature difference between the two faces of that surface. The volumetric heat capacity represents the capacity of a material to store thermal energy. These two properties are of extreme importance in heat conduction problems.

Currently, there are several techniques in order to determine the thermophysical properties of the most diverse materials. These techniques can determine the properties separately or simultaneously, in addition, most of them occur quickly, safely and accurately (Jannot *et al.*, 2006, Jannot *et al.*, 2009, Xamán *et al.*, 2009, Jannot *et al.*, 2010). The hot-plate method presented around 1910 is normalized by ABNT (2005) and is cited as the most accurate method to estimate the thermal conductivity of insulating materials (Ribeiro *et al.*, 2004). Blackwell (1954) presented the hot-wire method that is currently widely applied to the determination of the thermal conductivity, since the experimental

equipment is simple. Developed by Parker *et al.* (1961), the flash method is used to estimate thermal diffusivity by applying a radiant heat pulse with high intensity and short duration on a surface of the analyzed sample.

Two models for simultaneous estimation of λ and ρc_p are presented in this paper. For the first model (M1), a thermal model based on the equation of the one-dimensional transient diffusion in Cartesian coordinates is used. A uniform heat flux is imposed on the top surface of a homogeneous sample, while the bottom surface ($x = L$) is isolated. The properties are estimated from a least square minimization, which function is defined by the square of the difference between the experimental and numerical temperatures. The experimental temperature is measured by positioning a thermocouple on the surface opposite to the heating. Regarding the numerical temperature, the data is obtained by the solution of the thermal problem using the method of finite differences with implicit formulation. For the second model (M2), a different proposed model, it receives a cold plate to maintain the bottom surface at a constant temperature. This model was developed to be used in materials with elevated thermal diffusivity because the temperature is controlled and high heat fluxes can be imposed on it. For this model, the thermal properties were also obtained by using a least square minimization, but with simulated experimental and numerical data. The simulated experimental temperature is a synthetic data and was obtained by the addition of residual in the numerical data. To ensure unidimensionality, for both models, side surfaces much larger than thickness have been used, and the total time of the experiment/simulation is short. A symmetrical assembly is used, where the sample is located between the resistive heater and the insulation/cold plate.

The first thermal model has already showed its accuracy in Ramos *et al.* (2016) and Carollo *et al.* (2016). In this paper the results of the insulated model (M1) are presented with experimental and numerical data and the results of the cold-plate model (M2) are presented with simulated experimental and numerical data.

Synthetic data are generally generated and used to prove some theoretical mathematical model comparing the behavior of the data generated synthetically with those obtained by the model (Ayala-Rivera *et al.*, 2013). The generation of synthetic data is a technique of statistical disclosure control (SDC). It is applicable to several fields of study and their systems, since the system has as characteristic the ability to simulate a theoretical scenario. Then, it can be verified if this system is satisfactory or not in the analysis of the phenomenon being studied. For this reason, the method aims to generate data from the original data using models that reproduce the structure of the original data as closely as possible (Viana, 2014).

An analysis of the sensitivity coefficients, which are defined by the partial temperature derivative with respect to the parameter to be estimated, was also done. This analysis is fundamental for the estimation of properties, since it allows to determine the best region to estimate each thermal property (that with the highest sensitivity coefficients), the correct positioning of the temperature sensor, the total time of the experiment, among other important parameters.

Therefore, the objective of this work is to present a comparison study between two thermal models in the simultaneous estimation of thermal conductivity and volumetric heat capacity of AISI 304 stainless steel.

2. METHODOLOGY

2.1 Thermal models

The first one-dimensional thermal model consists of a sample located between a resistive heater and the insulation, as shown in Fig. 1. To guarantee the unidirectional heat flux the analyzed sample has a much smaller thickness compared to the other dimensions. In addition, all surfaces of the sample, except the heated ($x = 0$), were isolated.

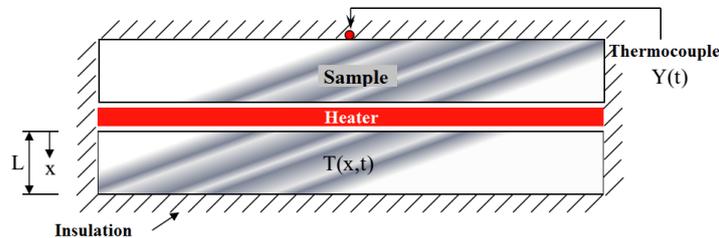


Figure 1. One-dimensional thermal model with insulation at $x = L$ (cross-sectional view).

The heat diffusion equation, considering the condition of constant properties, which describes the problem presented in Fig. 1 can be written as in Eq. 1:

$$\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{\rho c_p}{\lambda} \frac{\partial T(x,t)}{\partial t} \quad (1)$$

subjected to the boundary conditions:

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

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

and with the initial condition:

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

where x is the Cartesian coordinate, t is the time, ϕ is the imposed heat flux, T_0 is the initial body temperature and L is the thickness of the sample.

The new model, which consists of a sample located between a resistive heater and a cold plate, is now presented (Fig. 2). To guarantee the unidirectional heat flux the analyzed sample has a much smaller thickness compared to the other dimensions. The side surfaces of the sample were isolated, the top surface ($x = 0$) was heated with a uniform flux and the bottom surface ($x = L$) was maintained at a constant temperature of 15 °C.

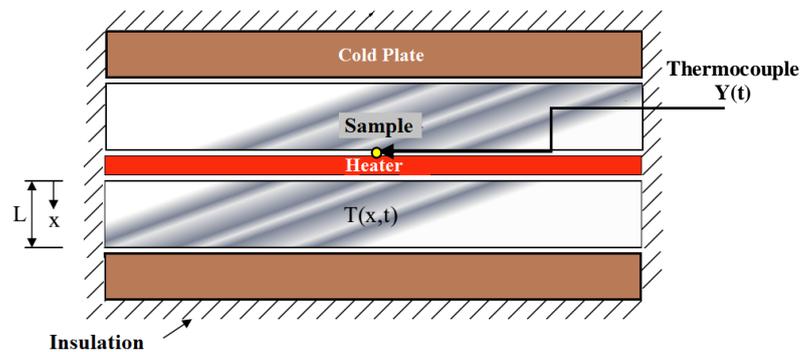


Figure 2. One-dimensional thermal model with constant temperature at $x = L$ (cross-sectional view).

For this model, the boundary condition at $x = L$ and the initial condition change:

$$T(x,t) = 15 \quad \text{at } x = L \quad (5)$$

$$T(x,t) = 15 \quad \text{at } t = 0 \quad (6)$$

2.2 Sensitivity Coefficients

The study of the sensitivity coefficients contributes to determine the ideal configuration of the experiment to estimate the properties. This study provides information such as the correct positioning of the thermocouples, the time of the tests, the time interval of the incidence of the imposed heat flux and the increase of time for the reading of the temperatures. The higher the value of the coefficients, the better the possibility of obtaining the properties reliably, but the difference between them should not be large, in order to avoid problems such as optimization by only one property.

The sensitivity coefficient is defined as the first partial derivative of the temperature in relation to the parameter to be analyzed (λ and ρc_p), written as follows in Eq. 7:

$$X_{ij} = P_i \frac{\partial T_j}{\partial P_i} \quad (7)$$

where T is the temperature calculated numerically, P is the parameter to be analyzed (λ or ρc_p), i the counter for the number of parameters and j the counter for the number of points. In this work we determine λ and ρc_p , we have: $i = 1$ for λ and $i = 2$ for ρc_p .

2.3 Broyden–Fletcher–Goldfarb–Shanno Method

To perform the estimation of the thermal properties analyzed, an objective function must be defined, which basically considers the experimental/simulated experimental temperature and the numerical temperature. In this way, this function is defined as the square of the difference between the experimental/simulated experimental and the numerical temperatures. Therefore, we have the following equation:

$$F = \sum_{j=1}^m (Y_j - T_j)^2 \quad (8)$$

where m is the total number of points, Y is the experimental/ simulated experimental temperature and T is the numerical temperature.

Then, it is known that the optimal value for λ and ρc_p , that is, the value that minimizes the objective function (Eq. 8) is the value of the property to be estimated. To obtain this value, it can be used optimization techniques. This work uses the BFGS (Broyden-Fletcher-Goldfarb-Shanno) optimization technique which is presented in Vanderplaats (2005). This technique is a particularity of the Variable Metric Methods. Because it is a first-order method, it is necessary to know the objective function gradient. The advantages of this method are the fast rate of convergence and the ease of working with numerous design variables.

2.4 Experimental Prodedure

The experimental bench is presented in Fig. 3 and it was used to perform the thermal properties estimation using the insulated model (M1). The computer is responsible for controlling the acquisition of data, which in turn collects the temperature data using a thermocouple positioned on the surface opposite to the heating ($x = L$). The direct current source is connected to the resistive heater and the multimeter used to measure the current imposed on the heater. All the assembly is wrapped by a thermal insulation material, in this case the polystyrene (styrofoam).

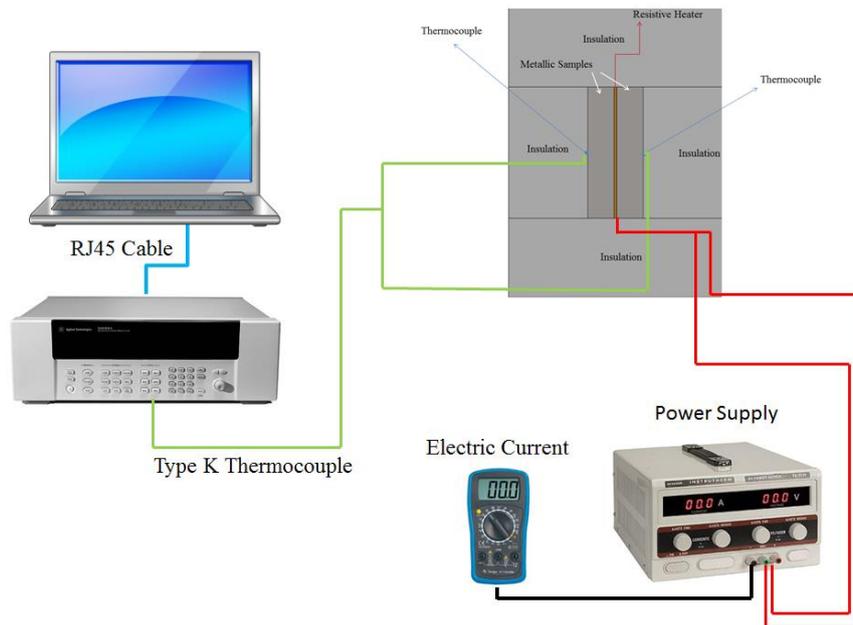


Figure 3. Experimental bench used for the insulated model.

A resistive heater was put between two samples of AISI 304 stainless steel. The resistive heater was fed by a power supply in way to get the heat needed to perform the experiment. By the way the heat intensity changes over experiment time in a way to get better sensitivity coefficients.

The samples of AISI 304 stainless steel analyzed have the following dimensions: 99.80 mm x 99.80 mm x 8.30 mm. The scale magnitude of these dimensions was determined to improve the one-dimensional condition of the heat flux imposed on the sample, with a minimum ratio of 1:5 being recommended. The sample was rectified to ensure a better contact surface, reducing the incidence of air gaps, which may interfere with the prescribed heat flux condition.

It was used a Kapton[®] (polyimide film) resistive heater with a resistance of 9.9Ω and with dimensions of $98.50 \text{ mm} \times 98.50 \text{ mm} \times 0.20 \text{ mm}$. It is used such a heater because the sample has a thickness that allows a uniform heating throughout its surface in a short period of time, according to Omega (2000).

After some tests, the heat fluxes imposed in the experiments were: first, 6860 W m^{-2} and, later, 1815 W m^{-2} .

2.5 Simulated Experimental Procedure

Simulated data are generally used to validate some theoretical mathematical model, analyzing the behavior of simulated data with those obtained by the model (Ayala-Rivera et al., 2013). The generation of simulated data is a technique of statistical disclosure control (SDC) applicable to several fields of study and their systems, since the system has the capacity to simulate a theoretical scenario. Therefore, this system can be verified as satisfactory or not in the analysis of the phenomenon under study. For this reason, the method aims to generate simulated data (simulated experimental temperature) from the original data (numerical temperature) using models that reproduce the original data structure as much as possible (Viana, 2014).

For the cold-plate model (M2), the thermophysical properties were obtained using least squares minimization with simulated experimental and numerical temperatures. The simulated experimental temperature was obtained by the addition of random errors in the numerical data. In this step, random errors of the order of $\pm 0.1 \text{ }^\circ\text{C}$ were used.

In the simulations, a sample with dimensions $100.00 \text{ mm} \times 100.00 \text{ mm} \times 10.00 \text{ mm}$ was considered. The heat fluxes were selected from observing the behaviors obtained, besides the real possibility of using them experimentally in laboratory. Then, the heat fluxes imposed were: first, 7709 W m^{-2} and, later, 1854 W m^{-2} .

3. RESULTS AND DISCUSSION

Experimental, numerical and simulated experimental data were used for estimating the thermal properties of the stainless steel AISI 304. Regarding the insulated model, where experimental and numerical data were used, in Fig. 4a there are the experimental and numerical temperature distributions on the surface $x = L$, and also the heat flux imposed on the surface $x = 0$. The temperatures increase at a strong rate at the beginning when there is a higher heat flux and continue to rise, but with less intensity until the end of the experiment.

X_1 represents the sensitivity coefficient for λ and X_2 for ρc_p . X_1 is multiplied by a factor to improve the visualization of the curve. For the first model, in Fig. 4b, it can be seen that X_1 increases during the first 10s, decreases, then remains constant; and X_2 increases proportionally with the temperature, then its value increases all over experiment time.

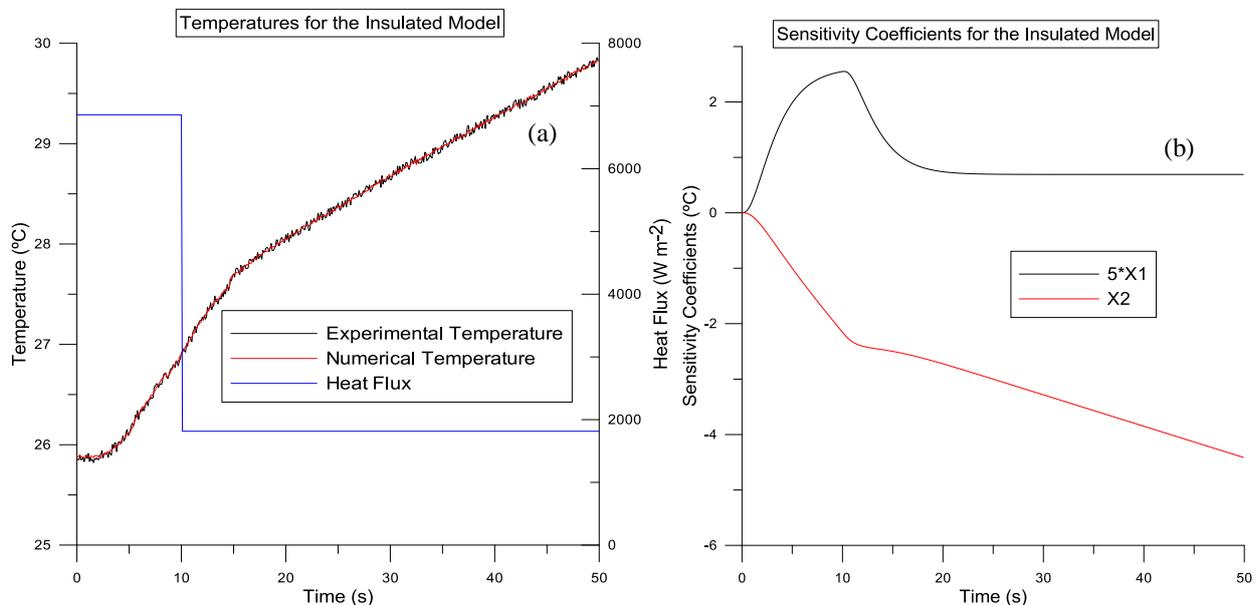


Figure 4. Insulated Model. (a) Numerical and Experimental Temperatures; (b) Sensitivity Coefficients.

Ten experiments were performed using the insulated model and the results obtained are presented in Tab. 1. In Tab. 2, the statistical values of the results and their comparison with the literature are presented.

Table 1. Values obtained for AISI 304 stainless steel using the insulated model.

Experiment	λ (W/mK)	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)
1	15.7202	4.3211
2	15.7162	4.3190
3	15.7156	4.3162
4	15.7200	4.3177
5	15.7188	4.3146
6	15.7193	4.3208
7	15.7204	4.3167
8	15.7191	4.3182
9	15.7174	4.3154
10	15.7188	4.3200

Table 2. Statistical values obtained for AISI 304 stainless steel using the insulated model.

Thermal property	Average	Standard Deviation	Borges <i>et al.</i> (2006)	Difference (%)
$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	4.3108	0.0021	3.89	9.2
λ (W/mK)	15.7186	0.0016	14.64	6.9

In relation to the cold-plate model, in Fig. 5a it is noted that the temperatures at $x = 0$ do not exceed 18.5 °C and that the temperature distributions lose amplitude and decrease shortly after the reduction of the intensity of the prescribed heat flux.

About the sensitivity coefficients, in Fig. 5b, X_1 has almost the same behavior as the previous model, but it reaches higher values, since the heat flux used in this model is better absorbed by the sample, because the presence of the cold plate drains the heat without risk of overheating the sample; the behavior for the sensitivity coefficient of ρc_p is a bit different from that seen earlier for the insulated model because the temperature decreases strongly due to the presence of the cold plate. Then, since X_2 is intrinsically bound to the temperature, its values are reduced.

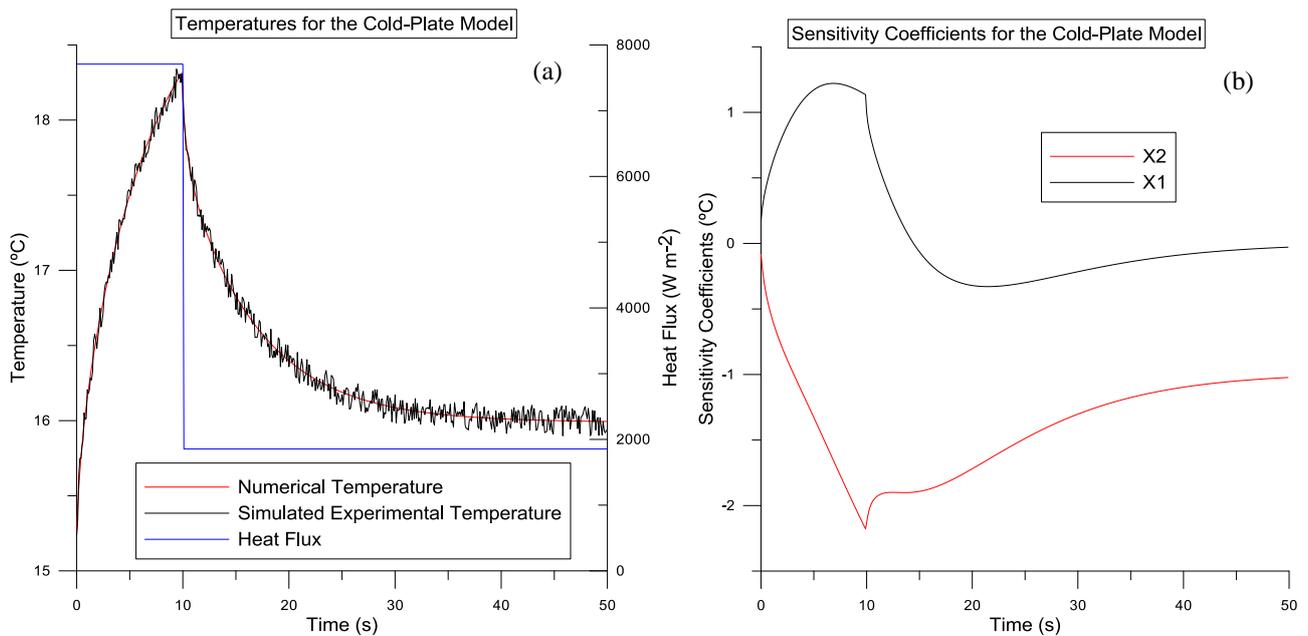


Figure 5. Cold-plate Model. (a) Numerical and Simulated Experimental Temperatures; (b) Sensitivity Coefficients.

For the cold-plate model, simulated experimental and numerical data were used. Thus, 10 simulations were made with the addition of a random error of ± 0.1 °C at the temperature obtained numerically. The results of the simulations are presented in Tab. 3 and in Tab. 4 there are the statistical values for such results, as well as their comparisons with the reference.

Table 3. Values obtained for AISI 304 stainless steel using the cold-plate model.

Simulation	λ (W/mK)	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)
1	16.1222	4.2312
2	16.1251	4.2297
3	16.1302	4.2317
4	16.1255	4.2401
5	16.1217	4.2355
6	16.1288	4.2289
7	16.1263	4.2299
8	16.1301	4.2352
9	16.1227	4.2406
10	16.1234	4.2366

Table 4. Statistical values obtained for AISI 304 stainless steel using the cold-plate model.

Thermal property	Average	Standard Deviation	Borges <i>et al.</i> (2006)	Difference (%)
$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	4.2339	0.0041	3.89	8.1
λ (W/mK)	16.1256	0.0030	14.64	8.9

It is clear to see that the cold-plate model reaches temperatures much lower than those taken for the insulated model. In this case, the temperature rises little with the first heat flux, also having a low amplitude, and falls rapidly with the change of heat fluxes, coming close to the temperature maintained constant in the cold plate.

The sensitivity coefficients are higher for the cold plate model, showing another advantage of this thermal model, besides the possible application of high heat fluxes without the risk of overheating the sample under analysis.

4. CONCLUSIONS

Both models presented good sensitivity coefficients, showing that the technique used has efficacy. Both the isolated model and the cold plate method were effective, with the first one offering more accurate in the estimation of thermal properties, comparing to Borges *et al.* (2006). However, it has to be noted that both models are statistically equivalent, that was observed in a statistical significance and equivalence test. The cold plate model, in turn, is preferable in the estimation of λ , since it allows the use of high heat fluxes, as it does not allow a sample to overheat. High heat fluxes in the insulated model would cause it to reach high temperatures, making it difficult to use common insulating materials such as polyvinyl chloride and expanded polystyrene.

Future works concern a deeper analysis of the best regions to estimate the thermal properties, using an experimental assembly for the cold-plate, which is expected to be made soon, and 3D thermal models. Then, it will possible to compare both models using experimental data.

5. ACKNOWLEDGEMENTS

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