

A DIFFERENT APPROACH FOR THE THERMAL PROPERTIES SIMULTANEOUS ESTIMATION OF MANY MATERIALS BASED ON SENSITIVITY COEFFICIENTS

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Abstract. *This work presents a method for the simultaneous estimation of thermal conductivity, λ , and volumetric heat capacity, ρc_p , in samples of Glass, AISI 304 Stainless Steel, AISI 1045 Steel, Iron, and Aluminum 5052. The thermal model used is based on transient one-dimensional diffusion equation. This model uses a constant and uniform heat flux on the top surface and insulation condition on the bottom surface, where the temperature is analyzed. Thus, the properties estimation was supported on analysis of the sensitivity coefficients defined by the first partial derivative of the temperature in relation to the parameter to be analyzed, times the analyzed parameter. Based on this analysis, two different intensities of heat flux were used: in order to increase the sensitivity coefficient for λ estimation, a higher intensity was applied at the beginning and to ensure enough sensitivity for ρc_p estimation a lower intensity was employed at the end. Another explanation for the use of two different values of the heat flux is that the intensity of the sensitivity coefficient cannot be much different for the properties; in other words, if one coefficient is much larger than the other, the estimation by using minimization will occur only for the property which presents the higher coefficient. Hence, the properties are simultaneously estimated, supported on these coefficients, which must show a global minimum value for each property besides having to be linearly independent. To estimate these properties, an error function defined by the square difference between the numerical temperature with random errors and numerical temperature is minimized by applying the optimization technique BFGS (Broyden-Fletcher-Goldfarb-Shanno). The numerical temperature is obtained by the solution of proposed thermal model using the Finite Difference Method with an implicit formulation. After several numerical analyses by using simulated data, the maximum difference found were 0.29 % for the thermal conductivity and 0.12 % for the volumetric heat capacity when obtained properties were compared with the literature. A contribution of this work is the study of the global minimum value in set with the sensitivity coefficients, because sometimes the sensitivity is not enough to determine the properties with accuracy.*

Keywords: *thermal properties, heat conduction, optimization, sensitivity coefficients, global minimum.*

1. INTRODUCTION

Nowadays, due to globalization, more and more new techniques are required to quickly, reliably and accurately determine the thermophysical properties of materials. These techniques can estimate the properties simultaneously and non-simultaneously. Another important aspect is the economic issue, because the lower the cost to determine the parameters, ensuring reliability, the greater the chance to compete in the national and international markets. The technique proposed in this paper can be used, for example, to correctly choose, under the point of view thermal properties, the materials to be used in the manufacture of a heat exchanger. This choice is made by taking into account the values of thermophysical properties, which should be ideal to yield a saving that is directly linked to energy and environmental issues, widely discussed in the current global circumstances.

Another example can be a machining process which great part of the heat generated by friction between the workpiece and the cutting tool must be transferred to the tool holder, as the tool wear is directly linked to temperature increase. Thus, the right tool for the process can be chosen through the knowledge of its thermal conductivity, λ , since this property determines the range of the working temperature of the material. From these needs, researchers have developed many techniques which are being improved continuously (Carvalho *et al.*, 2006 and Brito *et al.*, 2009).

There are three methods frequently used to estimate thermal properties: the Guarded Hot Plate, Hot Wire Technique, and the Flash Method. The Guarded Hot Plate Method (ASTM C177, 1997) which is widely used to determine λ of insulating materials is considered by many researchers as Wulf *et al.* (2005) and Lima *et al.* (2008), among others, the most accurate and reliable. In this method, the homogeneous and isotropic sample, in shape flat plate is placed between a hot and a cold plate in such a way that the heat flux through the central area of the sample is unidirectional. Under steady state conditions, the thermal conductivity is calculated by measuring the heat flux and the mean gradient of temperature on the sample. The Hot Wire Technique presented by Blackwell (1954) became widely used to determine the thermal conductivity. This technique is basically performed by inserting a cylindrical probe which contains a resistance wire and a thermocouple in the middle of a sample. This method can also be used to obtain the thermal diffusivity, α , requiring for this, the application of another thermocouple on the sample. A restriction to this method concerns about metallic materials due to high contact resistance between the probe and the sample, since it is very

difficult to avoid the air gaps present in the assembly. Several researchers have improved this technique in order to determine the properties of other materials (Nahor *et al.*, 2003 and Adjali and Laurent 2007). The former optimized the position of the hot wire to find food conductivity, and the latter proposed a change in methodology to determine the conductivity of a water-agar gel mixture by varying the temperature. The Flash Method developed by Parker *et al.* (1961) is used to determine the thermal diffusivity. This technique consists of applying a radiant heat pulse of great intensity and short time on a surface of a sample. It is then possible to obtain the thermal diffusivity based on the time required for the temperature on the other side to reach the maximum value. A limitation to determine the thermal conductivity in this technique is the need to know the amount of energy absorbed on the front face of the sample. Since this is a widely researched topic, new methods have been developed to eliminate the limitations of the above techniques (Shibata *et al.*, 2002, Santos *et al.*, 2005 and Coquard and Panel 2008).

From this point other techniques used to determine the thermal properties will be presented. These techniques are used to determine the properties simultaneously or not simultaneously for many materials.

Taktak *et al.* (1993) determined λ and volumetric heat capacity, ρc_p , simultaneously for a carbon fiber and epoxy compound. The assembly consisted of a square-shaped sample with prescribed heat flux condition on the top surface, and prescribed temperature on the opposite surface. The temperatures were monitored on both sides. This study aimed to demonstrate the ideal conditions to perform the experiment in order to achieve reliable and accurate results. Seeking to find the best study area to obtain the properties, an analysis of the sensitivity coefficient and the determinant was carried out. The criteria chosen for this analysis were: position of the thermocouple in relation to the heater, the time experiment, and the heating. Thus, they concluded that to obtain more accurate results, it is feasible to collect the temperature as close as possible to the heat flux and to heat up the sample to be investigated in the shortest possible time.

Dowding *et al.* (1995) used a sequential technique in transient experiments to determine λ and ρc_p simultaneously for a carbon-carbon compound. The symmetrical assembly consisted of a heater placed between two samples isolated by a non-conductor ceramic plate. This work was developed for the one-dimensional thermal model to study the influence of the position of the thermocouples on the sample by analyzing the sensitivity coefficients. The properties were estimated by varying the temperature from room temperature to 623 °C using a controlled atmosphere furnace.

Blackwell *et al.* (2000) proposed the determination of λ in the transient state. To achieve this goal, the sensitivity coefficients were analyzed to guide the design of an experiment to estimate the thermal conductivity for the steel AISI 304. The conductivity was determined by an experimental setup, where the heat conduction was considered axial on the walls of a hollow cylinder.

Borges *et al.* (2006) presented a method to obtain simultaneously and independently α and λ for conductive and non-conductive materials. One advantage of this technique refers to the fact of obtaining the properties simultaneously, but independently, since two objective functions were applied: one in a frequency domain and another in the time domain. The frequency domain function was obtained by calculating the phase of the response function of a dynamic system, and the time domain function was based on known temperatures. A disadvantage of this study is the small number of points to estimate α and how it is estimated first, since this may influence the results of λ .

Jannot *et al.* (2006) developed a Transient Hot Plate Method to determine simultaneously the thermal effusivity, b , and the thermal conductivity of metallic materials such as aluminum, titanium and steel. The proposed device uses a simple heating element inserted between a plane face sample of the material to be characterized and a sample of an insulation material. The heating element and the sample have the same area so that the heat transfer may be considered as unidirectional as long as the convective heat losses are negligible. Temperature sensors were used in order to estimate the properties by minimizing a quadratic error function between the experimental and numerical temperatures. Sensitivity studies were realized to determine the best region to analyze the properties as well as the ideal thickness of the sample. One disadvantage of this study is the large thickness of the samples, which increases the cost.

Ghrib *et al.* (2007) developed a method based on the Mirage Effect, which is possible to estimate simultaneously α and λ of metallic materials like aluminum, steel, titanium, among others. The method is based on the comparison of the amplitude variation and of the phase of the experimental thermal sign with the square root of the modular frequency. The properties were estimated when the experimental and theoretical temperature curves were coincident. The values of the estimated properties were in good agreement with the literature values. The disadvantage of this method is the high cost of the experimental apparatus.

Thomas *et al.* (2010) presented a different experimental design to determine the three components of the thermal conductivity tensor and the specific heat of polymer composite materials. This method is based on the sensitivity coefficients and the properties were estimated by using an inverse method. The advantage of this work is to use a heater which has micro-thermocouples incorporated inside it, allowing measurement of the temperatures. However, this method can be only used to determine the thermal properties of materials which presented thermal conductivity up to 10 W/mK.

In the present work a method is proposed to determine simultaneously the thermal conductivity and the volumetric heat capacity for many materials, from isolated to metallic, using the same experiment. This method is based on a one-dimensional heat conduction model and uses simulated data of heat flux and temperature. The heat flux had different intensities for each part of the experiment, in order to achieve the ideal conditions to estimate the properties in

according with the sensitivity coefficients analyses. The properties are estimated by minimizing the quadratic error function based on the difference between experimental and numerical temperatures. To minimize this function, the sequential optimization technique BFGS is used. The temperature is obtained by the numerical resolution of the heat diffusion equation for the thermal model by using the finite difference method with implicit formulation. Furthermore, analyses of the sensitivity coefficients along with the error function are performed to find the best setting and region to obtain the properties. This idea of doing a set analysis was developed after some results presented in Carollo *et al.* (2010a). In this work was observed that the procedure cited by many researchers presented sensitivity, but this sensitivity is not enough to determine simultaneously the properties with accuracy for metallic materials. In other words, it is very difficult to find the global minimum value for the error function, which corresponds to the correct thermal properties values, when metallic materials are analyzed.

Therefore, the objective of this work is to do a study with the purpose to extend the methodology proposed in Carollo *et al.* (2010b). Thus, it is possible to determine simultaneously the thermal conductivity and the volumetric heat capacity for many materials, from isolated to metallic.

2. THEORETICAL ASPECTS

2.1. Thermal model

Figure 1 shows the proposed one-dimensional thermal model, which consists of a sample located between a resistive heater and an insulator. To ensure the unidirectional heat flux, the sample has much smaller thickness than its other dimensions. In addition, all the surfaces, except the heated ($x = 0$), were isolated.

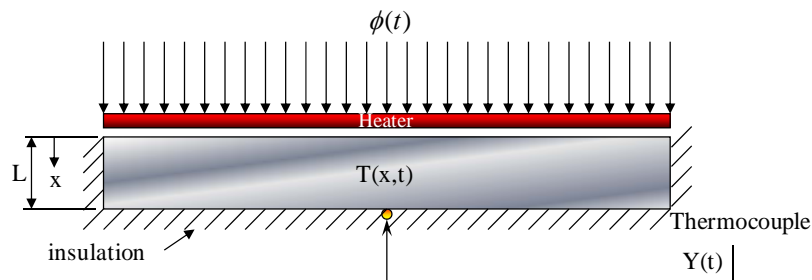


Figure 1. One-dimensional thermal model.

The heat diffusion equation for the problem presented in Figure 1, considering the thermal properties constant, can be written as:

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

subject to the boundary conditions:

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

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

and the initial condition:

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

where x [m] is the Cartesian coordinate, t [s] the time, ϕ [W/m^2] the prescribed heat flux, T_0 [$^\circ\text{C}$] the initial temperature of the sample and L [m] the thickness.

The temperature is numerically calculated through the solution of the one-dimensional diffusion equation using the finite difference method with an implicit formulation.

2.2. Analyses of the best region to determine the properties λ and ρc_p

Studies of the sensitivity coefficient for each sample are performed in this work in order to determine the ideal region to estimate the properties and the best configuration of the experimental setup. This study provides information such as: the correct positioning of the thermocouples, the experimental time, and the time interval of the applied heat flux incidence. The higher the coefficients value, the better the chance of obtaining the properties reliably.

The sensitivity coefficient is defined by the first partial derivative of the temperature in relation to the parameter to be analyzed (λ or ρc_p), being written as follows:

$$X_{ij} = P_i \frac{\partial T_j}{\partial P_i} \quad (5)$$

where T [°C] is the numerical temperature, P the parameter to be analyzed (λ [W/mK] or ρc_p [Ws/m³K]), i [-] the index of parameter, and j [-] the index of points. As in this work, only two properties will be analyzed, $i = 1$ for λ and $i = 2$ for ρc_p .

Besides this, analyses of the error function were done in order to guarantee that in the analyzed region there is enough information to estimate the properties simultaneously. One can verify this information if a minimum value of the function error is found when there are changes of the properties values. This error function is represented by Eq. (6) in the next section.

2.3. Thermal conductivity and volumetric heat capacity simultaneous estimation

To estimate the two properties it is necessary to use an error function based on the square difference between the experimental and numerical temperatures. This equation can be written as:

$$F = \sum_{j=1}^m (Y_j - T_j)^2 \quad (6)$$

where, m [-] is the total number of points, and Y (°C) the experimental temperature presented by Eq. (7). Thus, in this work the experimental temperature is obtained by using the numerical temperature with random errors.

$$Y_j = T_j + \varepsilon \quad (7)$$

where, ε [°C] is the random errors.

These random errors were based on the temperature residuals obtained from the results presented in Carollo *et al.* (2010b). The temperature residuals were around 0.25 % which corresponds to 0.05 °C. Therefore, the random errors adopted were ± 0.05 °C for all the simulations.

It is known that the optimal value for λ and ρc_p , in other words, the value that minimizes the error function, is the value of the property to be estimated. To obtain this value you can use optimization techniques, such as the BFGS (Broydon-Fletcher-Goldfarb-Shanno) sequential optimization technique used in this work, and presented in Vanderplaats (2005). This technique is a particularity of Variable Metric Methods. The advantages of this method are the fast convergence and the ease to work with many design variables.

3. SENSITIVITY AND ERRORS FUNCTIONS ANALYSES

The analyses were based on Carollo *et al.* (2010b), which presented an experimental procedure to determine the thermal properties of metallic materials, like AISI 304 Stainless Steel. In this work, many studies of the sensitivity coefficient along with the error function were done. In this sense, these analyses were used as a start up to extend this technique to obtain the thermal properties of a large range of materials, from 0.1 W/mK to 150 W/mK. Following, it can be seen the results for each material chosen.

3.1. Glass

The study was carried out by using the thermal properties values from Incropera *et al.* (2007). The thermal properties values used were: 1.38 W/mK for the thermal conductivity and 1.64×10^6 Ws/m³K for the volumetric heat capacity. The thickness sample is 10 mm. The simulation lasted 160 s, but the heat flux was imposed from 0 to 140 s. In the first part, that consist in the interval of 0 to 20 s, the applied heat flux was approximately 1000 W/m². For the second part, the time between 20 to 140 s, the imposed heat flux was around 460 W/m². The time interval used to monitor the temperature was 0.1 s. This configuration for the heat flux was chosen with the purpose to keep the temperature

difference less than 10 °C in order to guarantee the hypotheses of thermal properties constants adopted. It can be seen the temperatures and the applied heat flux in Fig. 2. Besides to keep the temperature difference less than 10 °C, this procedure was done, because it is necessary to control the magnitude relation between X_1 (sensitivity coefficient for λ) and X_2 (sensitivity coefficient for ρc_p), to assure that the estimation will happen for the two properties; in other words, if one coefficient is much larger than the other, the estimation, by using minimization, will occur only for the property which presents the higher coefficient.

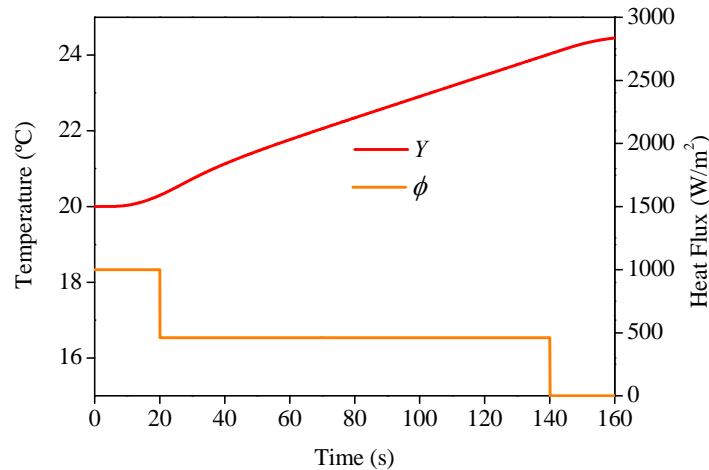


Figure 2 – Temperature at $x = L$ and applied heat flux at $x = 0$.

The sensitivity analysis was performed for two reasons: to determine the best region to estimate the properties, in other words, to choose the points that will be analyzed in the minimization and to determine the better intensities of the applied heat flux. In addition, these coefficients have to obey the condition of being linearly independents, because if they are linearly dependents, it is impossible to determine the thermal properties simultaneously. Analysis of the error function was done along with to sensitivity analysis in order to guarantee that there was enough influence to determine these properties in the selected region. Figure 3 shows the sensitivity coefficients at $x = L$ for λ and ρc_p , and Fig. 4 presents the values of the error function for each property. The points selected to be analyzed corresponds to the period of applied heat flux. As you can see, for the points chosen it is possible to determine the thermal properties simultaneously, because there is a global minimum value for each property analyzed.

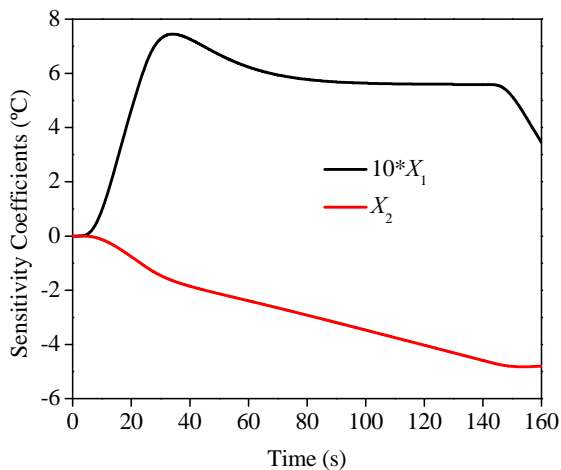


Figure 3 – Sensitivity coefficients at $x = L$.

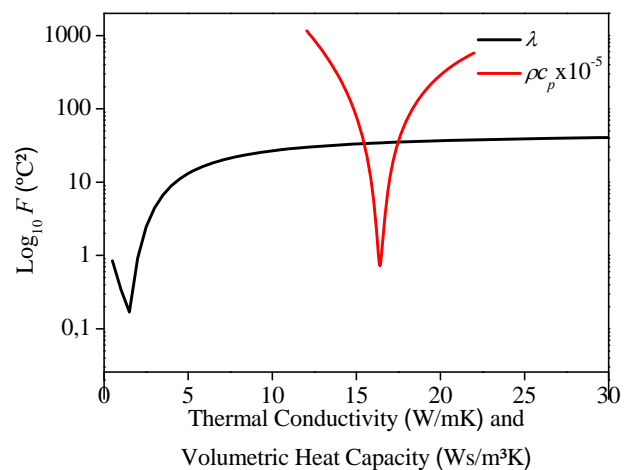


Figure 4 – Error function for each property.

3.2. AISI 304 Stainless Steel

This analysis was done similarly to Glass. In this simulation, 160 s were analyzed, but the heat flux was applied during the 140 s. The increment of time used was the same used for the Glass (0.1 s). The applied heat flux was 2640 W/m^2 for the first part (0 to 20 s), and 660 W/m^2 for the second part (20 to 140 s). The thermal properties values, from Carollo *et al.* (2010b), are: 14.61 W/mK and 3.91×10^6 Ws/m^3K and the sample present a thickness of 10 mm. Figure 5 presents the temperature and the applied heat flux, Fig. 6 presents the sensitivity coefficients at $x = L$ and Fig. 7 presents the error function.

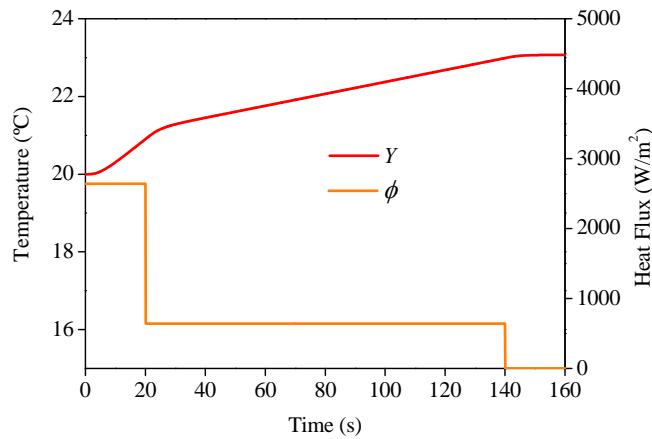


Figure 5 – Temperature at $x = L$ and applied heat flux at $x = 0$.

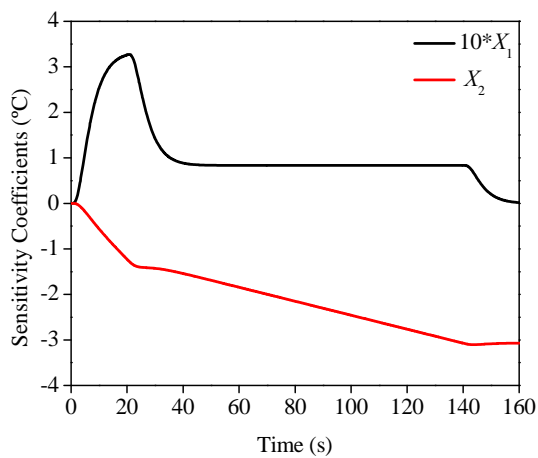


Figure 6 – Sensitivity coefficients at $x = L$.

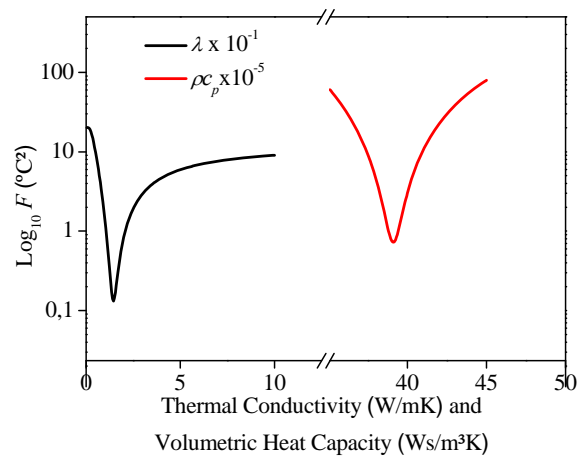


Figure 7 – Error function for each property.

3.3. AISI 1045 Steel

This part presents the simulation for the AISI 1045 Steel. The simulation was carried out by using the thermal properties values of 49.80 W/mK and 3.82×10^6 Ws/m³K from Incropera *et al.* (2007) and following the procedure used to Glass. The thickness sample is 15 mm. The simulation lasted 160 s, but the heat flux was imposed from 0 to 140 s. In the first part, that consist in the interval of 0 to 20 s, the applied heat flux was approximately 10000 W/m². For the second part, the time between 20 to 120 s, the imposed heat flux was around 2500 W/m². The time interval used to monitor the temperature was 0.1 s. Figure 8 presents the temperature and the applied heat flux, Fig. 9 presents the sensitivity coefficients at $x = L$ and Fig. 10 presents the error function.

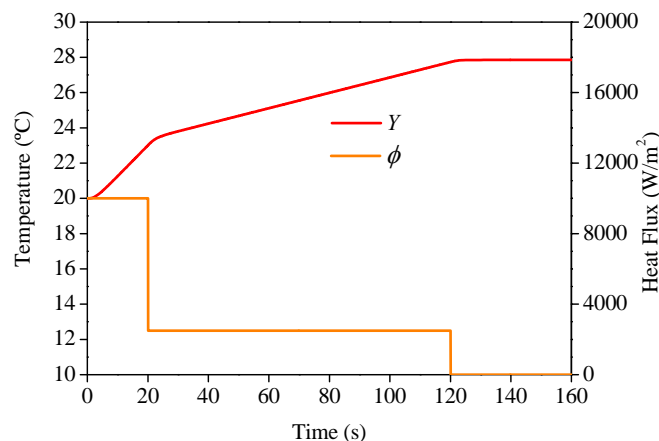


Figure 8 – Temperature at $x = L$ and applied heat flux at $x = 0$.

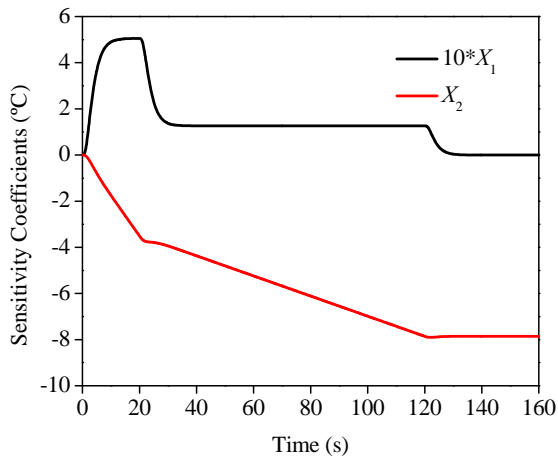


Figure 9 – Sensitivity coefficients at $x = L$.

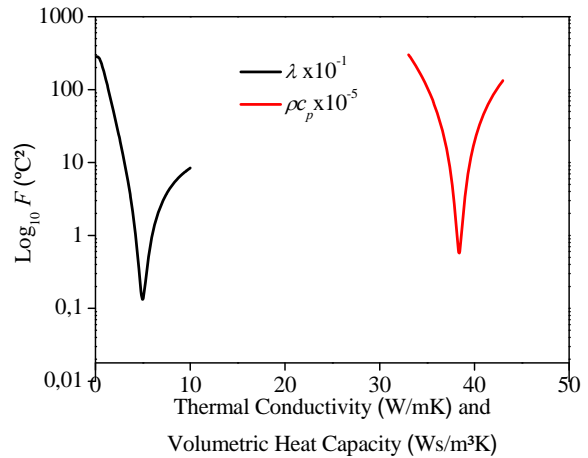


Figure 10 – Error function for each property.

3.4. Iron

For the iron the analysis was done similarly to the other materials and the thermal properties were found in Incropera *et al.* (2007). In this simulation, 160 s were analyzed, but the heat flux was applied during the 120 s. The increment of time used was 0.1 s. The applied heat flux was 12000 W/m² for the first part (0 to 20 s), and 3000 W/m² for the second part (20 to 120 s). The thermal properties values are: 76.20 W/mK and 3.46x10⁶ Ws/m³K and the sample present a thickness of 17 mm. Figure 11 presents the temperature and the applied heat flux, Fig. 12 presents the sensitivity coefficients at $x = L$ and Fig. 13 presents the error function.

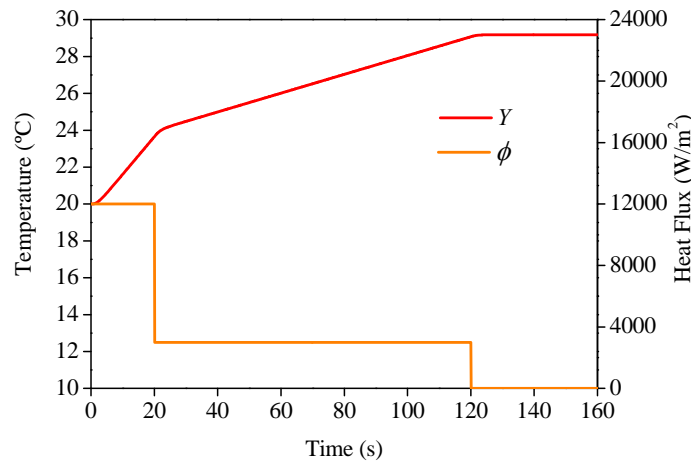


Figure 11 – Temperature at $x = L$ and applied heat flux at $x = 0$.

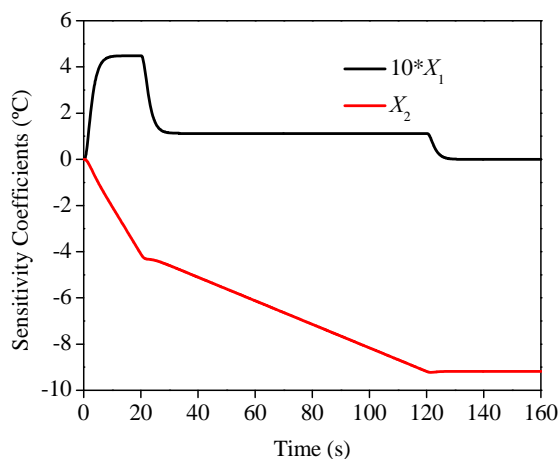


Figure 12 – Sensitivity coefficients at $x = L$.

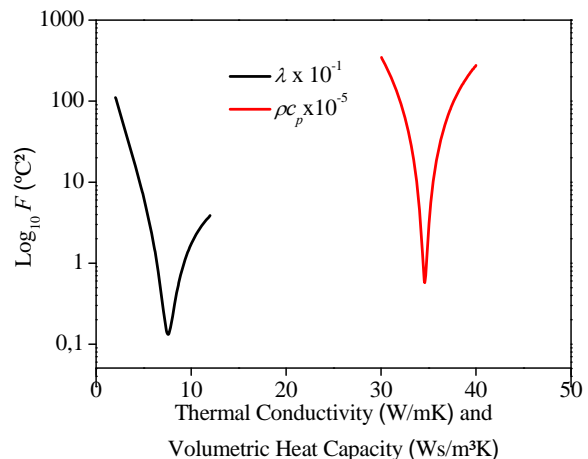


Figure 13 – Error function for each property.

3.5. 5052 Aluminum

This part presents the simulation for the 5052 Aluminum. The simulation was carried out by using the thermal properties of 137.00 W/mK and 2.45×10^6 Ws/m³K from MatWeb (2011) and following the procedure used to Glass. The thickness sample is 20 mm. The simulation lasted 160 s, but the heat flux was imposed from 0 to 100 s. In the first part, that consist in the interval of 0 to 20 s, the applied heat flux was approximately 12500 W/m². For the second part, the time between 20 to 120 s, the imposed heat flux was around 2350 W/m². The time interval used to monitor the temperature was 0.1 s. Figure 14 presents the temperature and the applied heat flux, Fig. 15 presents the sensitivity coefficients at $x = L$ and Fig. 16 presents the error function.

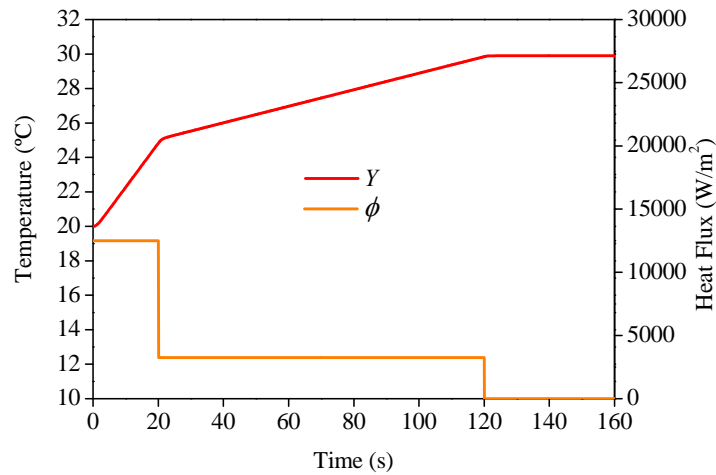


Figure 14 – Temperature at $x = L$ and applied heat flux at $x = 0$.

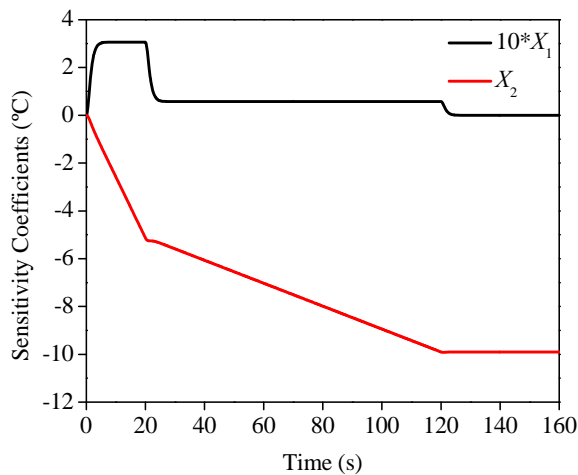


Figure 15 – Sensitivity coefficients at $x = L$.

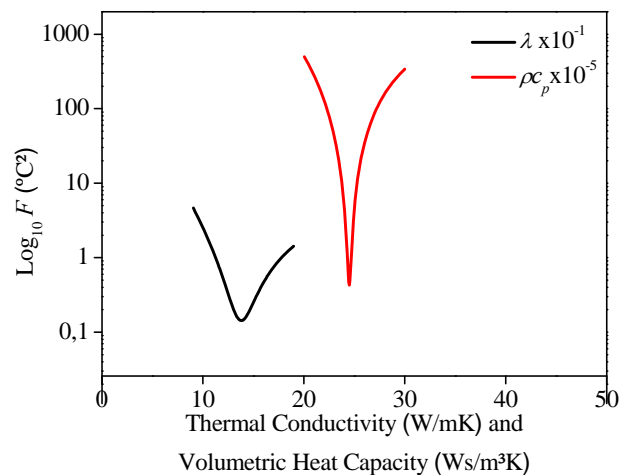


Figure 16 – Error function for each property.

3.6. Comments

All the simulations were done as an attempt to obtain the sensitivity coefficients similarly to the AISI 304 Stainless Steel sensitivity coefficients. Another point is to obtain the global minimum value for each property. Thus, to achieve these conditions, the intensities of heat flux, thickness, experimental time, heat flux duration and others were modified. As you can see, all the sensitivity coefficients presents the same way, but with different intensities; however, the properties could be estimated for all materials and the results are in good agreement with the literature.

It can be seen that the thickness of the samples changed for each material. Nevertheless, when the thickness increases, the other dimensions have to increase proportionally. In order to guarantee the condition of unidirectional heat flux, it was decided to use the following dimensions for the each material: Glass (50x50x10 mm), AISI 304 Stainless Steel (50x50x10 mm), AISI 1045 Steel (100x100x15 mm), Iron (100x100x17 mm) and Aluminum 5052 (100x100x20 mm).

4. RESULTS ANALYSIS

For each material ten (10) simulations were carried out to estimate the thermal properties simultaneously. For each simulation a different random errors were used to calculate the experimental temperatures. These analyses were carried out using the same procedure to verify if the results are equivalents. In addition, to be sure that the results are reliable, the first guess was modified for each simulation. Thus, all the simulations presented similar results.

Table 1 presents the obtained mean results of the present work, the literature value or reference and the difference for all analyzed materials. This percentage difference is calculated by the difference between the mean value of the present work and the literature value divided by the literature value. It can be seen goods results obtained for all materials.

Table 1 – Results obtained for all materials.

Material	Property	Present work	Reference	Difference (%)
Glass	λ (W/mK)	1.376	1.38	0.290
	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	1.641	1.64	0.061
AISI 304 Stainless Steel	λ (W/mK)	14.620	14.61	0.068
	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	3.908	3.91	0.051
AISI 1045 Steel	λ (W/mK)	49.488	49.80	0.016
	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	3.822	3.82	0.052
Iron	λ (W/mK)	76.194	76.20	0.008
	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	3.464	3.46	0.116
5052 Aluminum	λ (W/mK)	137.230	137.00	0.167
	$\rho c_p \times 10^{-6}$ (Ws/m ³ K)	2.449	2.45	0.041

Analyzing the sensitivity coefficients for the thermal conductivity, it can be seen that its intensity depends on the thermal conductivity of the material. Thus, a material which has low thermal conductivity present higher sensitivity coefficient than a material has a higher thermal conductivity, considering the same conditions. Thus, this is the reason of applied heat flux on the aluminum sample to be higher than on glass sample. Another point is the thickness of the material, because the larger the thickness, the larger is the sensitivity coefficient. Therefore, this is the justification for the aluminum thickness is the largest and the glass thickness the lowest. Still analyzing the sensitivity coefficients, X_2 increase almost equal to the temperature difference. Thus, it is very important to control the intensities of applied heat flux and the time duration in order to obtain a good sensitivity for ρc_p and to keep the temperature difference lower than 10 °C.

The error function analyses were done to guarantee that there is enough information to determine the thermal properties with accuracy. It can be seen that for all materials was find a global minimum value for each property, in others words, it is possible to determine the thermal properties in the analyzed points. It can be seen the global minimum value is more evident for ρc_p , than λ for some materials. An explanation for this behavior is the magnitude of the sensitivity coefficient, because the higher the sensitivity value, the higher is the precision of the thermal property estimation.

5. CONCLUSIONS

This paper presents a methodology to simultaneous estimate the thermal conductivity and the volumetric heat capacity of many materials, from 0.1 W/mK to 150 W/mK, applying different intensities of heat flux. Five materials were analyzed: Glass, AISI 304 Stainless Steels, AISI 1045 Steel, Iron and 5052 Aluminum. After several numerical analyses, the maximum difference found were 0.29 % for the thermal conductivity and 0.12 % for the volumetric heat capacity when obtained the thermal properties were compared with the literature. The contribution of this work is to extend the technique presented in Carollo *et al.* (2010b) for other materials. The next step is to prepare an experimental apparatus and to carry out the experiments in laboratory to validate the methodology and to propose this methodology to determine the thermal properties by varying the initial temperature.

6. ACKNOWLEDGEMENTS

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