THE USE OF CFX AND INVERSE TECHNIQUES FOR THE ESTIMATION OF HEAT FLUX AND TEMPERATURE

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Abstract. *This paper presents a comparison between two Inverse Problems techniques to solve inverse heat transfer problems. The Function Specification is the first, and the second is a technique which applies optimization algorithms. Both these techniques use the commercial software CFX to solve differential equation by using Finite Volume Method. These simulations are based on one and three-dimensional controlled experiment carried out in laboratory using AISI 304 Stainless Steel sample. Symmetrical assemblies were performed in both cases, in order to ensure the correct measuring of the applied heat flux value. Furthermore, the assemblies were completely isolated by polystyrene plates. Thermocouples were inserted on many surfaces in order to measure experimental temperature. In next step, the heat flux applied by those two techiniques was estimated. After obtained the estimated heat flux, simmulations were performed with theses estimated flux to calculate the temperatures on equivalent monitored experimentals points. According to the Function Specification results, this technique presents good results for estimated heat flux and calculated temperatures through this heat flux; on the other hand, the technique which involve optmization algorithm did not presented good results for the estimated heat flux, however presents an excellent result for the temperature.*

Keywords*: Inverse problems, heat conduction, Function Specification, CFX, optimization.*

1. INTRODUCTION

Daily, it can be countless situations subject to heat transfer. A reliable knowledge of heat transfer rates and temperature levels is an essential condition to control, improve, and develop any process where heat transfer occurs. New methods called Inverse Techniques were developed to meet the demands for high-energy efficiency allied to the need for easier methods to measure temperatures in many phenomena. Inverse Techniques are tools that allow the measuring of certain parameters indirectly through the use of other variables. Among the several uses of the applications of Inverse Problems one can mention the temperature measurements on the tool rake face and combustion engine chamber.

The information available from the system does it to be considered direct problem or inverse problem. A problem is called direct when knows previously its boundary and initial conditions, otherwise, it face to an inverse problem. Direct problems have advantage in to be equated easier than inverse problems. However direct problems are hard to solve without know previously initial and boundary conditions. In practice is very usual unknown precisely those conditions, due to impossibility to instrument correctly the system. Inverse problems independent on previous knowledge of boundary condition of system to be analyzed, however requires a more elaborated modeling that can requires more computational processing power than direct problems. This characteristic does inverse problems techniques excellent to analyze heat transfer problems on complex geometries bodies; whereas the sensor can be put on an easier access region and the data are measured in order to estimate the real interest variable on point which cannot be measured directly. As example of inverse problems applications can be cited determination of heat flux applied on cutting tool on machining process, estimation of temperature in a metallurgical process, further heat flux applied on blast furnace bricks.

Beck *et al.* (1985) was one of the first in develop inverse problems techniques. There are several inverse problems techniques. According to Özisik and Orland (2000), this classification is based on nature of heat transfer process that can be conduction, convection, radiation or still a combination of those. Furthermore, heat transfer process can be one-dimensional or involve more dimensions. Inverse problems techniques always have as aim minimizing an objective function, which, in this case, is the difference between estimated and actual value of interest variable.

Inverse problems solutions often involve numerical methods, as finite elements, finite volume among others. It is also known, that geometry affects temperature distribution and heat transfer. Therefore, some researchers have sought gather inverse problems techniques with commercial software as CFX. The advantage is versatility in might modeling various geometries, as well readiness in to accept any boundary condition , since the most simple, which occurs only heat transfer by conduction to more complex conditions including natural and forced convection effects and radiation.

Several research have carried out studies on this, among them, Huang and Chen (1999) who implemented the use of CFX 4.2 software with an inverse problem technique called Conjugate Direction Method, in order to study forced convection heat transfer, in transient regime in ducts. Years later Huang and Lo (2005) has studies temperature in cutting tools. In this work, software CFX 4.4 was applied together inverse problem technique. This software was used to solve heat diffusion equation, while error between estimated and experimental temperatures was minimizes through Steepest Descent Method. Huang *et al.* (2007) have estimated heat flux on drilling tools for titanium drilling through inverse problems techniques applied with software CFX 4.4.

This work has as goal, to compare two inverse problems techniques for one and three dimensional heat conduction cases. One of these techniques is the Function Specification and other uses Fletcher Reever optmization algorithm. Both are used together CFX 12 software. In this work the inverse problems techniques are used to estimate the heat flux applied for one and three dimensional cases, while CFX are used to solve the diffusion heat equation by finite volume method and obtain the temperatures field on the sample. The methodology is validated with experiments carried out in laboratory. On one-dimensional experiment, entire AISI 304 Stainless Steel upper surface was uniformly heated by resistive heater, while remaining surface are insulated. On other experiment, to assure three- dimensional heat conduction condition, another AISI 3304 Stainless Steel, was submitted to resistive heater only in part of upper surface, being remaining surface insulated.

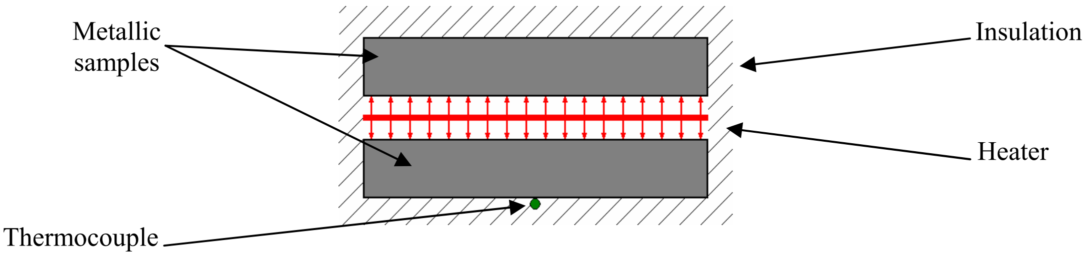
In the future, intend apply this methodology in cutting tools for turning machining process. Machining process is strongly dependent on cutting tool performance, which in turn, is affected in function of the thermal field which is subjected during turning machining process. In consequence of this, the thermal field analysis of cutting tools for machining process has attracted attention from numerous researchers as Tay *et al.* (1976), Stephenson (1991), Stephenson (1996), Jen *et al.* (2001), Battaglia *et al.* (2005), Singamneni (2005), Carvalho *et al.* (2006) and Dogu (2006). The techniques that have been used to analyze temperature fields in machining process include experimental methods and simulations with numerical calculations. Experimental studies use thermocouples and infrared cameras, while numerical techniques generally apply finite elements or finite volumes among others techniques. Thus, inverse problems techniques, due its own characteristics, can be implemented in machining process in order to known these temperature gradients, since this is essential to develop tools, improve process even reduce costs.

2. THEORETICAL ASPECTS

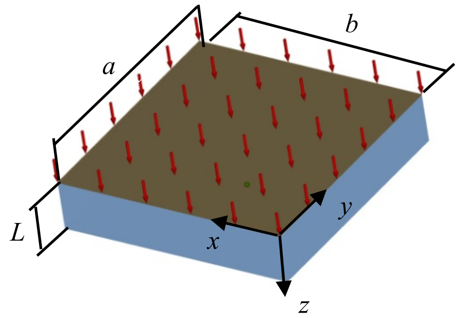
In the next are presented thermal models approached on analysis proposed in this paper.

2.1. The one-dimensional thermal model.

Figure 1 presents the thermal problem scheme for one-dimensional model. A homogeneous sample of AISI 304 stainless steel initially at T_0 is subjected to an uniform and constant heat flux, q_0'', on the top surface, while all the others surfaces are insulated. It is observed on Fig. 1a that the thermal model is presented in a symmetrical assembly. The symmetrical assembly is used in order to reduce errors on the measurements of the applied heat flux. Figure 1b presents one-dimensional model detailed view. In this figure, the variables *a*, *b* e *L* are, respectively length, width and thickness of AISI 304 Stainless Steel sample.



(a)



(b)

Figure 1. (a) One-dimensional symmetrical assembly. (b) AISI 304 Stainless Steel sample details.

The heat diffusion equation, in Cartesian coordinates, for the presented problem in Fig. 1 is given by:

$$\frac{\partial^2 T}{\partial z^2}(z,t) = \frac{1}{\alpha}\frac{\partial T}{\partial t}(z,t) \tag{1}$$

subject to the following boundary conditions:

$$-\lambda \frac{\partial T}{\partial z}(z,t) = q_0^{"} \text{ at } z = 0 \tag{2}$$

$$-\lambda \frac{\partial T}{\partial z}(z,t) = 0 \text{ at } z = L \tag{3}$$

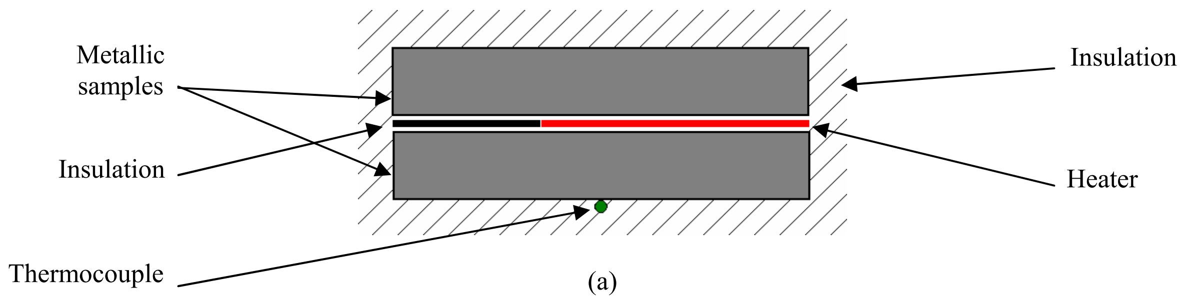
and the initial condition:

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

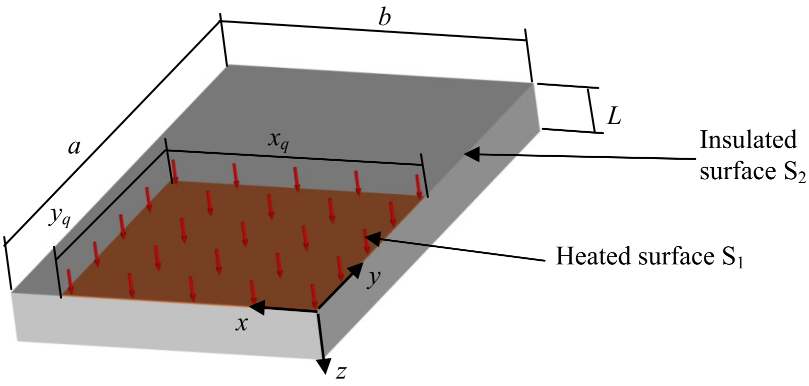
where T_0 is the initial temperature, t the time, α the sample thermal diffusivity, λ the sample thermal conductivity and z the Cartesian coordinate.

2.2. The three-dimensional thermal model

Figure 2 shows the design for three-dimensional thermal model. This model uses a homogeneous sample of AISI 304 stainless steel subjected to an uniform and constant heat flux, $q_0^{"}$. In this case, the heat flux is applied only in part the upper surface, from time t = 0. All the others surfaces are insulated. Thus, as in one-dimensional model, a symmetrical assembly is adopted.



(a)



(b)

Figure 2. (a) Three-dimensional thermal model. (b) AISI 304 Stainless Steel sample details.

As in the previous case, a and b are the samples length and width, x_q and y_q are the dimensions of the heated surface S_1 and furthermore insulated surfaces are called S_2. The heat diffusion equation, in Cartesian coordinate, is represented by Eq. (5):

$$\frac{\partial^2 T}{\partial x^2}(x,y,z,t)+\frac{\partial^2 T}{\partial y^2}(x,y,z,t)+\frac{\partial^2 T}{\partial z^2}(x,y,z,t)=\frac{1}{\alpha}\frac{\partial T}{\partial t}(x,y,z,t) \tag{5}$$

subject to the following boundary conditions:

$$-\lambda\frac{\partial T}{\partial z}(x,y,0,t)=q_0^{"} \text{ at } S_1,\ (0\le x\le x_q,\ 0\le y\le y_q) \tag{6}$$

$$-\lambda\frac{\partial T}{\partial z}(x,y,L,t)=0 \text{ at } S_2,\ (\ x,y\in S\,/(x,y)\notin S_1\ ) \tag{7}$$

$$\frac{\partial T}{\partial x}(0,y,z,t)=\frac{\partial T}{\partial x}(b,y,z,t)=\frac{\partial T}{\partial y}(x,0,z,t)=\frac{\partial T}{\partial y}(x,a,z,t)=\frac{\partial T}{\partial z}(x,y,0,t)=0 \tag{8}$$

and the initial condition:

$$T(x,y,z,t)=T_0 \text{ at } t=0 \tag{9}$$

being T_0 initial temperature, t time, α the thermal diffusivity, λ sample thermal conductivity and x, y and z the Cartesian coordinate. In this case, S represents the surface given by ($0\le x\le b$, $0\le y\le a$) and x_q, y_q and S_I surface boundaries, subject to applied heat flux.

2.3. The software CFX 12

After the models to be studied have been conceived, the next step is modeling them using the software CFX. This software allows to model geometries as well to configure boundaries and initial conditions. Thus, this software solve the heat diffusion equation for one and three-dimensional cases, applying Finite Volume Method. Finally, with CFX software the temperature field is obtained.

2.4. Function Specification

The heat flux components are used in algorithm of estimation in Sequential Function Specification method. An advantage of this method is the possibility to previously analyze the calculated and experimental temperature evolution according to number of future times adopted, to finally calculate the heat flux. This methodology aid in order to reduce the experimental noise spread in calculated heat flux. Other advantages are its easy implementation, low computational processing time if compared to others techniques. As disadvantage, cites appropriate functional (constant, parabolic, exponential or cubic) and future time value for estimation heat flux in time. The method consist assign a temporary functional shape for transient surface heat flux for in times over current of estimation. In this case, the shapes can be constant, parabolic, exponential or cubic. The simplest sequential procedure is which uses a sequence of straightlines segments as functional shape to describe the superficial heat flux behavior for future times. Thus, consider temporarily constant in time, several future heat flux components. The specified heat flux for r future times represents the flux model that will be estimated, in other words, the heat flux components (q_1, q_2, ..., q_{M-1}) are considered estimated previously and denoted by: $\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_{M+r-1}$. In order to increase the inverse algorithm stability, the heat flux components q_{M+1}, q_{M+2}, ..., q_{M+r-1} are assumed equal, $q_{M+1} = q_{M+2} = \ldots = q_{M+r-1}$ (Beck *et al.*, 1985). On q_M estimation sequential algorithm, the temperatures T_{M+1}, T_{M+2}, ..., T_{M+r-1} are necessary and them are calculated with hypothesis of constant heat flux. Thus, the q_M estimation is obtained through square difference minimization S among experimental temperatures (Y_{M+1}, $Y_{M+2,...,}$ Y_{M+r-1}) and calculated (T_{M+1}, T_{M+2}, ..., T_{M+r-1}), therefore:

$$S = \sum_{i=1}^{r} (Y_{M+i-1} - T_{M+i-1})^2 \tag{10}$$

where Y are experimental temperatures, T are calculated temperatures, M is the general index of time, r the future times value and i the future times counter.

2.5. Design optimization tool

This routine is an interface between an optimization algorithm and the software CFX. The optimization algorithm is a program in FORTRAN language that uses Fletcher Reeves algorithm optimization to estimate heat flux from experimental temperature. After estimated, the heat flux by program in Fortran, this is supplied to the CFX software to calculate the temperature distribution on the sample used in tests.

Figure 3 shows how this interface works between optimization algorithm in Fortran and CFX software. The routine in Fortran is an application of Fletcher Reeves optimization algorithm, to estimate the heat flux from experimental temperatures. The Fletcher Reeves algorithm is used on heat flux calculation in order to minimize an objective function, that, in this case, it is difference between experimental and estimated temperatures. The Fletcher Reeves algorithm is presented by Figure 4.

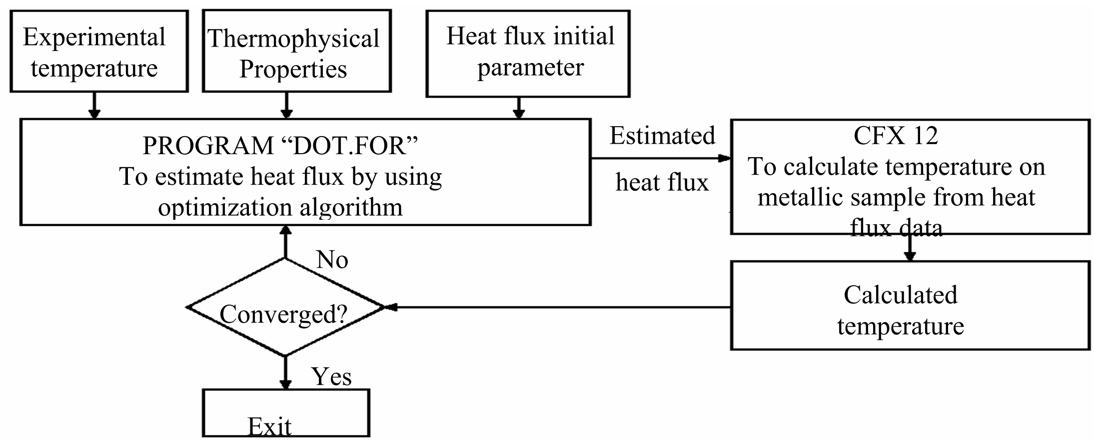


Figure 3. Computational routine used on experiments with AISI 304 Stainless Steel.

2.5.1 Fletcher Reeves optimization algorithm.

The Fletcher Reeves optimization algorithm or conjugate-direction is a first order optimization method. In first order method, is necessary to calculate the gradient of objective function, which does them more efficient than zero order method. Although the calculation of objective function gradient have to be done numerically, often with using numerical techniques such finite elements, the Fletcher Reeves algorithm is easy to implement and requires little computational storage.

Figure 4 below presents the algorithm. Note that is an algorithm similar to steepest descent method. However, the difference is in the iterations following the first, since this method has a better way to calculate the search direction, reducing the number of iterations needed for convergence.

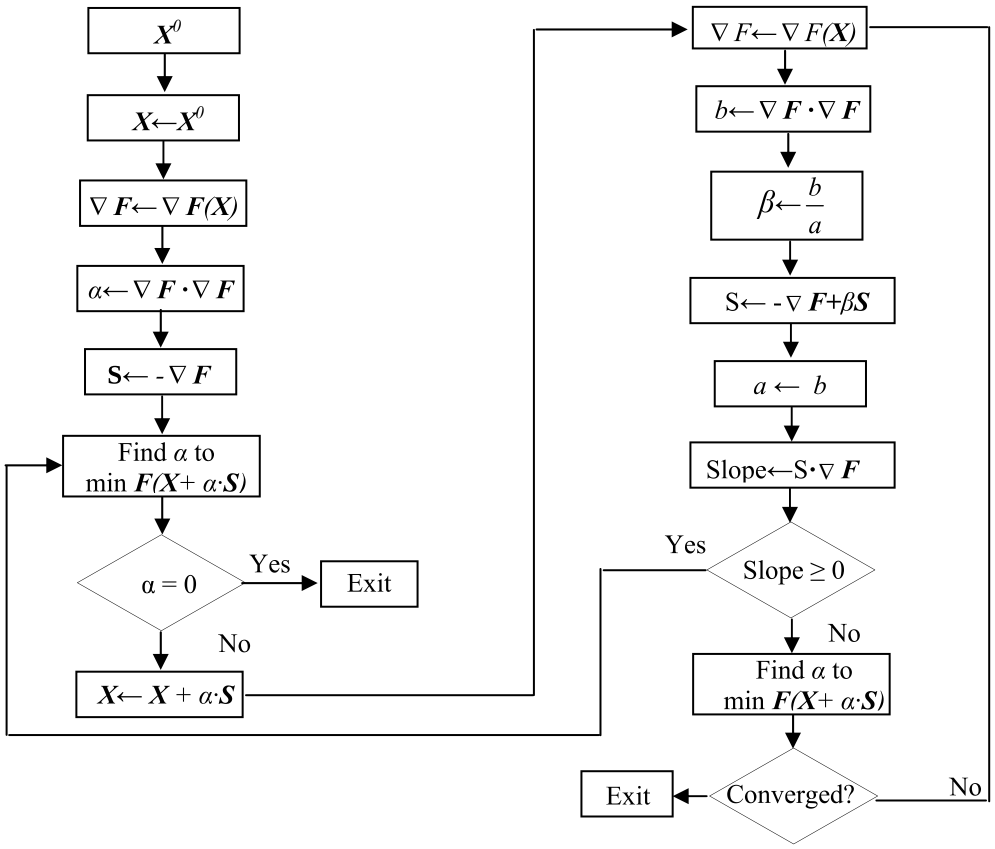


Figure 4. Fletcher Reeves optimization algorithm.

3. EXPERIMENTAL PROCEDURES

The experimental apparatus used is shown in Fig. 5. The AISI 304 Stainless Steel plates have the dimensions of 49.9 x 49.9 x 9.9 mm for one-dimensional case and 100.0 x 60.0 x 9.5 mm for three-dimensional case. The resistive kapton heater has a resistance of 15 Ω and the dimensions of 50.0 x 50.0 x 0.2 mm. The resistive kapton heater was used because it is very thin, allowing faster overall warming. This heater was connected to a digital power supply Instrutemp ST – 305D-II to provide the necessary heat flux. A symmetrical assembly was used to minimize the errors in the measured of the heat flux to be generated on the sample surface. The contact between the resistive heater and the sample is not perfect; therefore the silver thermal compound Arctic Silver 5 was used to eliminate the air interstices present in the assembly. The great advantage of this compound refers to its high thermal conductivity. In addition, weights were used on top of the isolated set samples-heater to improve the contact between the components. To minimize the effect of convection caused by the air circulating in the environment, the set samples-heater was isolated with polystyrene plates and it was put inside the oven. Temperatures were measured using thermocouples type K (30AWG) welded by capacitor discharge and calibrated using a bath temperature calibrator Marconi MA 184 with a resolution of ± 0.01 °C. The type K thermocouples were used to measure the temperatures on the opposite surface to heating. These thermocouple was connected to a data acquisition Agilent 34980A controlled by a microcomputer. In order to obtain better results, all experiments were performed in controlled room temperature. Figures 6a and 6b respectively show an expanded view for experiment for one and three-dimensional assembly. In these figures, it is seen as positioning the insulation, metallic samples and resistive heaters for each case.

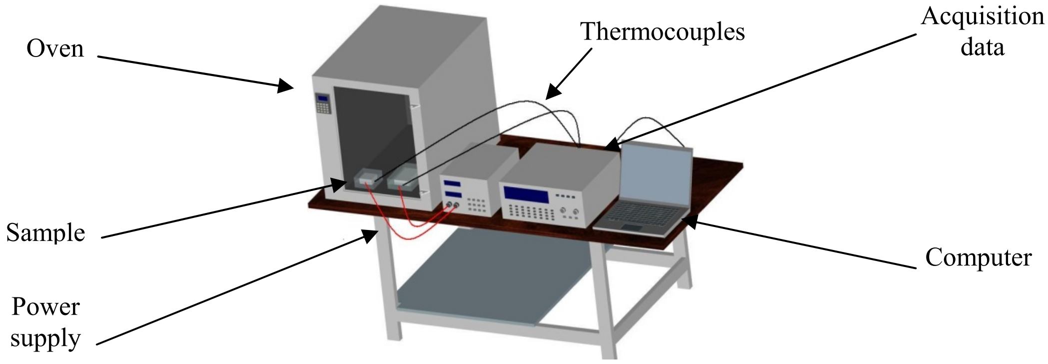


Figure 5. Sketch of experimental apparatus.

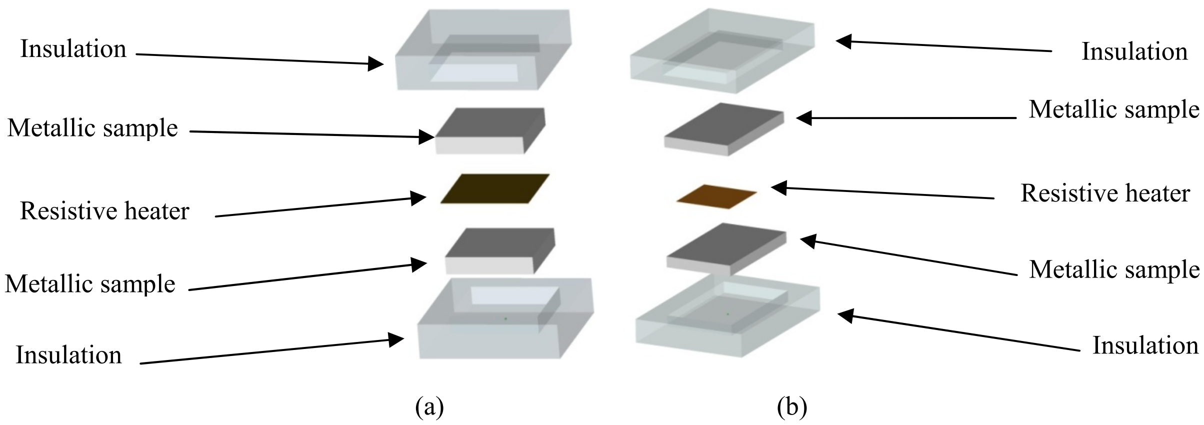


Figure 6. Sample assembly in details view.

Table 1 shows the thermophysical properties values adopted in this work. The value of the thermal conductivity was determined by Carollo (2010), whereas density and specific heat capacity were obtained from Incropera *et al*. (2007)

Table 1: Thermophysical properties adopted for AISI 304 Stainless Steel.

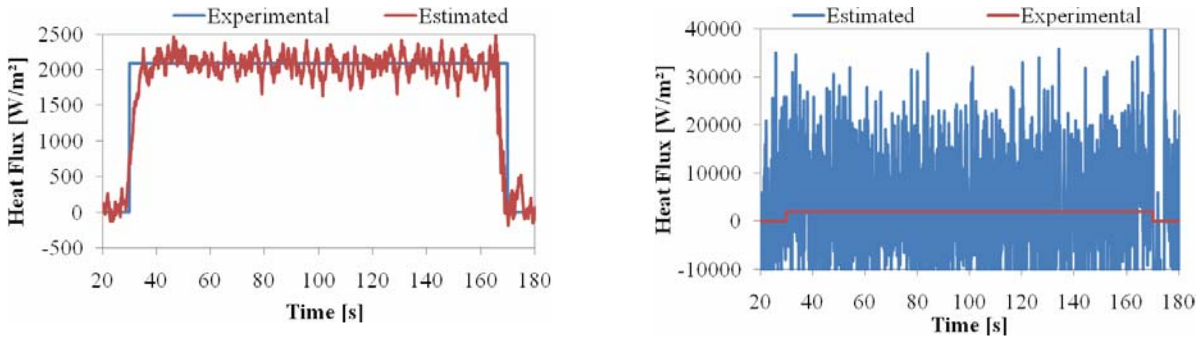
Properties	**Value**	**Unit**
Thermal Conductivity	14.574	W / mK
Density	7900	kg / m^3
Specific Heat Capacity	492.75	J / kgK

4. RESULTS ANALYSES

4.1 One-dimensional experiment

Thirty experiments were carried out for the one-dimentional model. Each experiment lasted 250 s, but the heat flux was imposed from 30 to 170 s. In the first part, that consist in the interval of 0 to 30 s, the applied heat flux was 0 W/m². In the middle part the applied heat flux was around 2535 W/m². Finally, the last 80 s were collected without heat flux. The time interval used to monitor the temperature was 0.1 s.

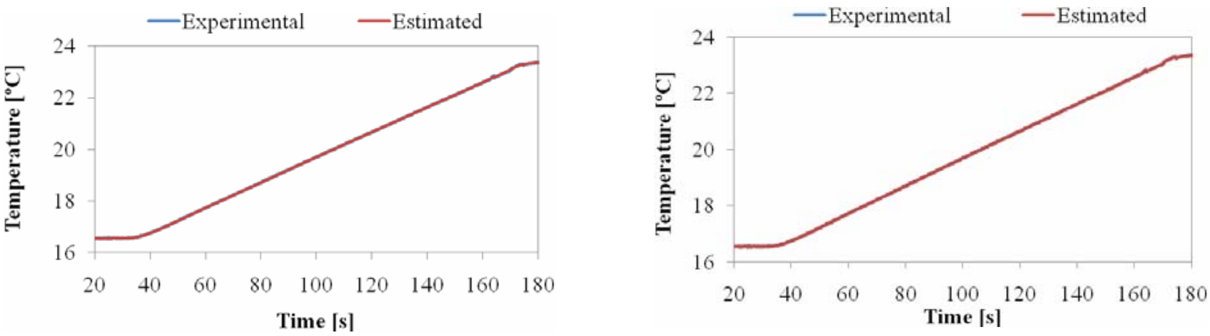
Figures 7a and 7b present a comparison between the estimated and experimental heat flux for one experiment. Since the results for the estimated heat flux from optimization technique have presented a higher deviation, the results are presented separately. In Figure 7a a comparison of the estimated heat flux from Function Specification technique with the applied heat flux is presented. The future times number of 50 was used for this technique. You can see that the mean value of the estimated heat flux is in agreement with the experimental heat flux. In Figure 7b the heat flux results obtained from the Fletcher Reeves technique are compared with the applied heat flux. In this case, the deviation is too large and this behavior is normal; however, in order to guarantee that this result is corrected, it is necessary to analyze the estimated temperature with this heat flux.



(a) (b)

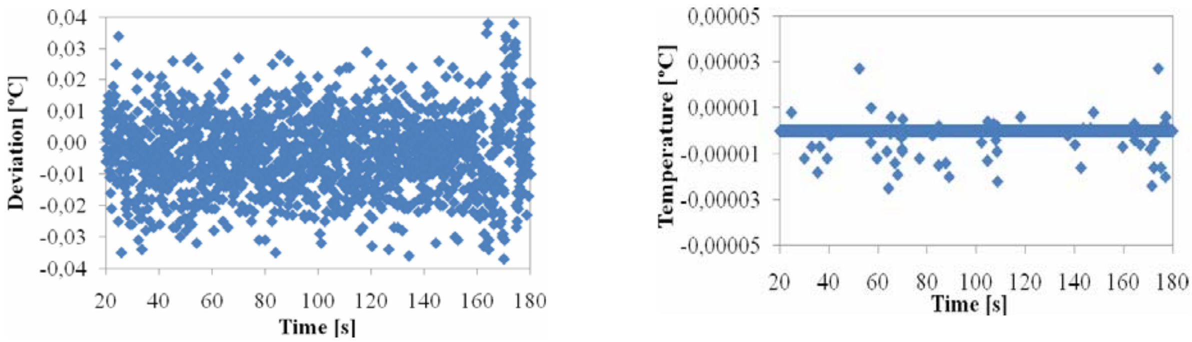
Figure 7. Comparison between estimated heat flux by Function Specification in (a) and Fletcher Reeves in (b).

Figures 8a and 8b show a comparison between the experimental and estimated values of temperature. The residuals between the estimated and experimental values of temperatures for each technique are presented in Figs. 9a and 9b. It can be seen in these figures that the maximum residual was obtained for the function specification technique and it was ± 0.3 ºC.



(a) (b)

Figure 8. Comparison between experimental temperatures and estimated temperatures from Function Specification method, in (a) and from DOT data, in (b).



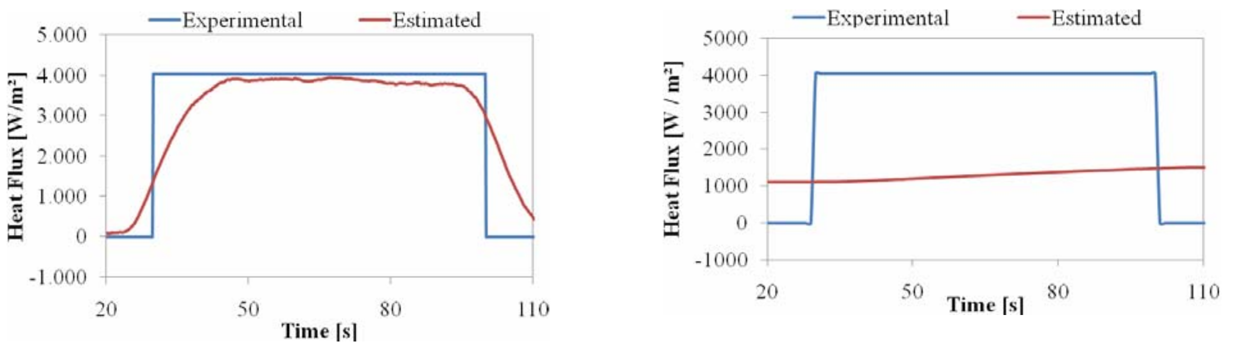
(a) (b)

Figure 9. Difference between experimental and estimated temperatures for Function Specification method in (a) and optimization algorithm in (b).

4.2 Three-dimensional experiment

For this case, ten experiments were carried out similarly to one-dimensional case. The heat flux was applied during the 70 s. The increment of time used to get the temperatures was the same used for the AISI 316 Stainless Steel (0.1 s). The applied heat flux was about 4037 W/m² for the second part (30 to 100 s), and 0 W/m² for the first and last part (0 to 30 and 100 to 150 s). Temperatures were taken on every 0.2 s. The thermophysical properties used on this case are the same used on one-dimensional case.

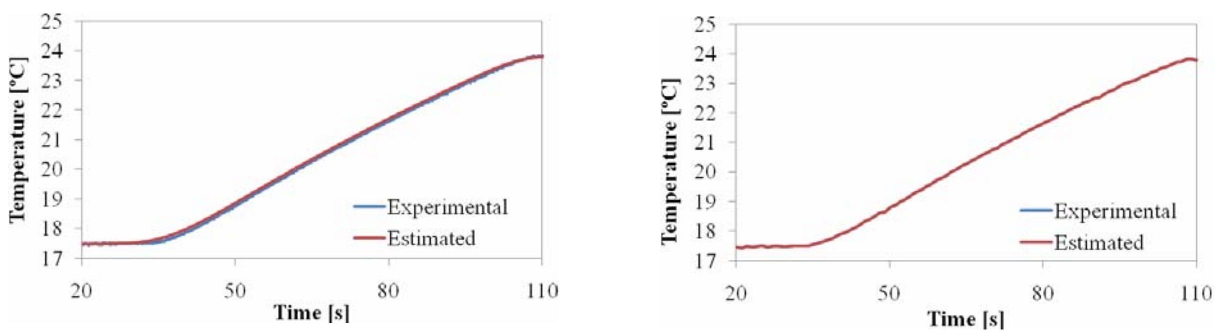
Figures 10a and 10b present a comparison between the estimated and experimental heat flux. As in one dimensional case, the Function Specification method has presented good results; however, the optimization technique have presents bad results. Due this, the comparison between experimental and estimated heat flux are presented separately. In Figure 10a a comparison of estimated heat flux from Function Specification technique with applied heat flux is presented. There was an average difference of 4.5 % between experimental and estimated heat flux. The future times number of 50 was used for this case too. In Figure 10b the heat flux results obtained from Fletcher Reeves technique are compared with experimental heat flux. For this model, the optimization technique has presented disagreement between experimental and numerical results. These bad results are due to a problem in the program which gets the results from the software CFX to calculate the heat flux. The authors are working in this program in order to solve this mistake.



(a) (b)

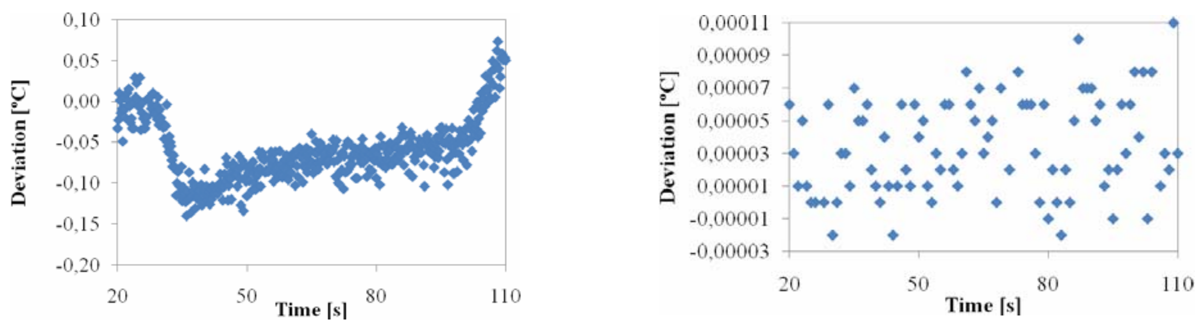
Figure 10. Comparison between estimated heat flux by Function Specification in (a) and DOT in (b).

Figure 11a and 11b show a comparison between the experimental and estimated temperature respectively. The Figs 12a and 12b shows the residuals between the estimated and experimental temperatures values of temperatures for each technique. It can be seen in these figures that the maximum residual was obtained for the Function Specification technique and it was ± 0.15 ºC.



(a) (b)

Figure 11. Comparison between experimental temperatures and estimated temperatures from Function Specification data, in (a) and from DOT data in (b).



(a) (b)

Figure 12. Difference between experimental and estimated temperatures for Function Specification method in (a) and optimization algorithm in (b).

5. CONCLUSIONS

It this work, the combined use of commercial software CFX and inverse problems techniques were proposed. The inverse techniques Function Specification and Fletcher Reeves were compared in one and three-dimensional heat conduction models. For the validation of the proposed methodology, the techniques of inverse problems were used in controlled experiments in laboratory. Good results were obtained, excepted for the heat flux from optimization algorithm. In this part there is an error in the program which is responsible to calculate the heat flux by using the temperature from the software CFX. Finally, the goal was achieve and this affirmation can be proved by analyzing the value obtained in this paper. For future, some improvements can be make like: to use more than one temperature signal simultaneously for Function Specification Technique, and to refine the interface between Optimization Algorithm and software CFX.

6. ACKNOWLEDGEMENTS

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7. REFERENCES

Battaglia, J. L., Puigsegur, L., Cahuc, O., 2005, "Estimated Temperature on a Machined Surface Using an Inverse Approach", Experimental Heat Transfer, Vol. 18, pp.13 – 25.

Beck, J. V., Blackwell, B. and St Clair, C., 1985, "Inverse Heat Conduction: Ill-podes Problems", Wiley – Interscience Publication, New York, 308p.

Carollo, L. F. S., Lima, G. M., Lima e Silva, A. L. F., Lima e Silva, S. M. M., 2010, "Estimativa Simultânea da Capacidade de Calor Volumétrica e da Condutividade Térmica de Materiais Metálicos", Submetido ao VI Congresso Nacional de Engenharia Mecânica - CONEM2010, Campina Grande, Paraíba, Brasil.

Carvalho, S. R., Lima e Silva, S. M. M., Machado, A. R., Guimarães G., 2006, "Temperature Determination at the Chip-tool Interface using an Inverse Thermal Model considering the Tool and Tool Holder", Journal of Materials Processing Technology, Vol. 179, pp. 97 – 104.

Dogu, Y., Aslan E., Camuscu, N., 2006, "A Numerical Model to Determine Temperature Distribution in Orthogonal Metal Cutting", Journal of Materials Processing Technology, Vol. 171, pp 1-9.

Huang, C. H., Chen, W. C., 1999, "A Three-Dimensional Inverse Forced Convection Problem in Estimating Surface Heat Flux by Conjugate Gradient Method", Int. Journal of Heat and Mass Transfer, Vol. 43, pp. 3171 – 3181.

Huang, C. H., Lo, H., 2005, "A Three-Dimensional Inverse Problem in Predicting the Heat Flux Distribution in the Cutting Tools", Numerical Heat Transfer, Vol. 48, pp. 1009 – 1034.

Huang, C. H., Jan, C. J., Li, R., Shih A. J., 2007, "A Three-Dimensional Inverse Problem in Estimating The Applied Heat Flux of a Titanium Drilling – Theoretical and Experimental Studies", International Journal of Heat and Mass Trasnfer, Vol. 50, pp. 3265 – 3277.

Incropera, F. P., DeWitt, D. P., Bergman, T. L., Lavine, A. S., 2007, "Fundamentals of Heat and Mass Transfer", John Wiley & Sons, 6th ed. USA, 997p.

Jen, T. C., Gutierrez, G., Eapen, S., 2001, Numerical Analysis in Interrupted Cutting Tool Temperatures", Numerical Heat Transfer, Vol. 39, pp. 1 – 20.

Özisik, M. N., Orlande, H. R. B., "Inverse Heat Transfer", Taylor & Francis, New York, 330p.

Singamneni, S. B., 2005, "A Mixed Solution for the Three-dimensional Temperature Distribution in Turning Inserts Using Finite and Boundary Elements Techniques", J. of Materials Processing Technology, Vol. 166, pp 98 – 106.

Stephenson, D. A., 1991, "Assessment of Steady-State Metal Cutting Temperature Models Based on Simultaneous Infrared and Thermocouple Data", Journal of Engineering for Industry, Vol. 113, pp. 121 – 128.

Stephenson, D. A., 1996, "Cutting Temperature of Ceramic Tools in High Speed Machining of Difficult-to-Cut Materials", International Journal of Machining Tools Manufacturing, Vol. 36, pp. 611 – 634.

Tay, A. O., Stevenson, M. G., Davist, G. V., Oxley, P. L. B., 1976, "A Numerical Method for Calculating Temperature Distributions in Machining From Force and Shear Angle Measurements", International Journal Machining Tool Design, Vol. 16, pp. 335 – 349.

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