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NUMERICAL TOOL FOR THE INVERSE ESTIMATION OF THE HEAT CAPACITY TEMPERATURE-DEPENDENT USING PSPICE

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ABSTRACT

In this paper a variant of the Sequential Function Specification Method has been used together with Network Simulation Method as the numerical method to solve an inverse problem associated with the determination of the heat capacity. It has been developed a software application for estimation the temperature dependence of heat capacity using the Qt platform and programming language Visual C++.

A set of temperatures measured at different points of the medium (obtained by means the numerical solution of the direct problem) and a random error affected by a normal distribution are used for evaluation of the classical functional that compares these temperatures with the temperatures obtained numerically at each step , and so an iterative least-squares approach function is obtained (heat capacity) by straight sections (piecewise function).

No prior information is used for the functional forms of the unknown specific heat, because this problem is considered a function estimation problem. A special device that generates a piecewise temperature-dependent function is required in conjunction with a programming routine.

The Network Simulation Method is the numerical method used, with a design of the network model easy and has very few electric devices. The software developed is used to run the network so that no mathematical manipulations are required. The effect of different parameters over the numerical solution has been studied. The results confirm that it is possible to estimate the heat capacity (or specific heat when the density is known) using experimental temperature history and a procedure inverse based in an iterative process.

INTRODUCTION

The heat transport in solid media is controlled by the thermophysical properties thermal conductivity and heat capacity or specific heat. When the thermal conductivity is constant, the two coefficients, along with the density, can be grouped into a single feature called thermal diffusivity. These properties have a determining influence on the temperature distribution and heat flux densities during transient processes of heating or cooling, which must be known distribution in numerous applications, for example, to design an optimal control of these processes. In most practical engineering problems, the thermophysical properties are temperature dependent, and therefore, the conduction equation is a partial differential equation whose solution is not linear, in general, is obtained through numerical techniques [1]. The inverse heat conduction problem is concerned with the determination of the thermal conductivity, the volumetric heat capacity, the initial condition, the boundary conditions and the heat sources using known temperature or heat flux. The inverse problems are more difficult than their corresponding direct problems because they are usually ill-posed. The estimation of the heat capacity which is a function of temperature is being considered in this study.

The estimate, therefore, of any of the thermophysical properties of a solid medium is a nonlinear inverse problem of enormous complexity, in any case much more difficult than the estimation of constant properties, or even that the estimation of time or space dependent properties. Needless to say, the interesting problem of simultaneous estimation of thermal properties from both of the measures taken in a single experiment, recently studied by some authors [2], is even more complex, requiring finer adjustments (for through a properly defined functional) to achieve a converged solution and valid.

In the scientific literature there are numerous publications, using different numerical techniques, estimate the thermal properties dependent on the temperature in the form of inverse problem. So [3] estimated the thermal conductivity temperature dependent; investigates the use of different locations for the measurement point temperatures and the influence of number of measures. Both elections significantly influence the estimate. Furthermore, [4] and [5] obtain estimates of the thermal property space. They determined the thermal conductivity in 1-D half with internal heat generation. Using two methods of solution based on finite differences in the first start from a continuous set of temperature measurements while the second uses a discrete set. Both methods can be applied to linear and nonlinear problems, without a priori knowledge of the type of dependence of the conductivity. Show three applications: conductivity constant, conductivity and position-dependent temperature-dependent conductivity. [6] using approximate analytical techniques based on the Laplace transform to estimate the thermal diffusivity of materials at high temperature in half dimensional. It contrasts the processes of cooling method for three materials, nickel, niobium and palladium, and studied the effect of error in measurements. [7] using an approximate method of direct integration performed simultaneous estimation of the thermal conductivity and heat capacity, both properties linear functions of temperature.

[8], using various measuring points, estimate the temperature dependency of conductivity and heat capacity in half 2-D orthotropic, using the iterative procedure based on Levenberg-Marquardt minimization of a functional characteristic. [9] estimated thermophysical properties by function estimation procedure, using the conjugate gradient method, and studying the effects on the estimate by modifying the position sensor measurements. [10] solved a function estimation problem of predicting temperature-dependent thermal conductivity without internal measurements [11] determined the temperature-dependent thermal conductivity in a stationary problem. [12] obtained a piecewise homogeneous function to estimate the thermal conductivity of conductors subjected to a heat flow test. [13] estimated the temperature-dependent thermal conductivity and heat capacity of manner simultaneous. [14] solved the inverse problem in simultaneously measurement temperature-dependent thermal conductivity and heat capacity.

The purpose of this paper is to propose a numerical software for determination of the heat capacity in order to obtain a response in temperature-stretches of the dependence with the temperature of the specific heat. Such a problem can be treated as one kind of the inverse heat conduction problem for a solid material. Transient temperature measurements at the boundary, from the solution of the direct problem, served as the simulated experimental data needed as input for the inverse analysis. Both direct and inverse heat conduction problems are solved using the network simulation method. The solution is obtained step-by-step by minimising the classical functional that compares the above input data with those obtained from the solution of the inverse problem. A straight line of variable slope and length is used for each one of the stretches of the desired solution.

Numerical tool employed has been the Network Simulation Method (NSM). This method rests on the electro-thermal analogy (loosely called the resistance-capacitance analogy or the RC analogy) that exists between the unsteady, unidirectional conduction of heat and the unsteady flow of electric current. Once the electric network model has been set up for the heat conduction equation, the numerical treatment of the analogy electric circuit equation can be easily done with the computer code Pspice.

NOMENCLATURE

c_o	[J/kgK]	Specific heat
C	[J/m^{3}K]	Heat capacity
C	[F]	Capacitor and capacitance
E	[-]	Voltage-control voltage-source
f_C	[-]	Mathematical function
F	[-]	Functional defined in eq. (10)
I	[A]	Current
k	[W/mK]	Thermal conductivity
L	[m]	Length
n	[-]	First value of temperature within the functional
N	[-]	Number of cells
R	[Ω]	Resistor
r	[-]	Number of terms of the functional
t	[s]	Time
T	[ºC]	Temperature
V	[V]	Voltage
x	[m]	Cartesian axis direction
Z	[-]	Number maximum of stretch
z	[-]	Particular number of stretch
Σ	[-]	Summation
Δ	[-]	Increment
∂	[-]	Differential
ΔC	[J/m^{3}K]	Deviation of the capacity heat in relation to the mean value
Δx	[m]	Thickness of the control volume
ΔT	[ºC]	Temperature interval associated to the functional
$\Delta\varepsilon$	[-]	Error percentage interval
ρ	[kg/m^3]	Density
ε	[-]	Random error value

Subscripts

DHCP	Direct problem
end	End
f	Particular location at the slab
ini	Initial
i	Associated to the volume element i, 1≤i≤N; also the centre of the volume element
IHCP	Inverse problem
i±Δx	Right and left ends of the cell elemental
j	1, 2, ..., p
L	Half a thickness of the slab mean value
max	Maximum
min	Minimum
n	Refers to the first temperature with the stretch
new	New
opt	Optimum
p	Natural number (total number of temperature measurements)
z	Number of stretch 1,2, ..., Z
0	Initial condition

MATHEMATICAL FORMULATION

The formulation of inverse heat conduction problem originates from the direct heat conduction formulation. For simplicity we assumed a medium one-dimensional and a cartesian coordinate system. Thus, for one-dimensional unsteady state heat conduction equation in a orthogonal coordinate, the direct formulations are as follows:

$$C(T)\,\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right), \quad \text{at } 0<x<L,\ t>0 \qquad (1)$$

$$k\,\frac{\partial T}{\partial t} = 0 \qquad \text{at } x=0,\ t>0 \qquad (2)$$

$$k\,\frac{\partial T}{\partial t} = q_L \qquad \text{at } x=L,\ t>0 \qquad (3)$$

$$T = T_o \qquad \text{at } t=0,\ 0<x<L \qquad (4)$$

$$C(T) = f_C(T) \qquad (5)$$

The direct problem, Equation (1) is concerned with the determination of temperature distribution T(x,t) in the interior region of the solid material as a function of time and position. In eq. (5) f_C defines an arbitrary continuous function of T.

The inverse problem arises if any of the parameters is not known especially $C=\rho c_e$ and k, but the transient temperature, boundary and initial conditions are known. The formulation of the IHCP involves Eqs. (1-4) and the set of temperatures $T_{IHCP}(x_f,t_j,\varepsilon_j)$ from the temperature measurement (or they can be obtained of the numerical solution of the direct problem DHCP and submitted to a random error ε_j). With this information, the aim is to obtained a approach solution of the dependence $C(T)$ by means of a piece-wise function in the form

$$C(T_z) = C_z \ (1\leq z \leq Z) \qquad (6)$$

This solution is defined by Z straight stretches of variable slope and size.

INVERSE DETERMINATION: ALGORITHM OF RESOLUTION

Discretizing equation (1) by method of finite difference [15].

$$C_i\,(dT_i/dt) = k\,(T_{i-\Delta} - 2\,T_i - T_{i+\Delta})/\Delta x^2 \qquad (7)$$

This expression can be expressed:

$$C_i\,(dT_i/dt) = [k\,(T_{i-\Delta} - T_i)/\Delta x^2] - [k\,(T_i - T_{i+\Delta})/\Delta x^2] \qquad (8)$$

At this moment the electrical analogy is applied and a network electrical circuit is designed. In this analogy: heat flux (q) and temperature (T) are connected to the electric variables current (I) and voltage (V), respectively. A number of volume elements N≥50, in 1-D geometry, ensures that the errors in the temperature and heat flux fields are around 0.5% in non-linear problems. The whole network, transformed into a lecture file, is solved by the computer code Pspice [16,17] using a PC.

Defining the currents:

$$I_{i,c} = \Delta x\, C_{i,}(T)\,(dT_i/dt \qquad (9a)$$

$$I_{i-\Delta x} = k\,(T_{i-\Delta x} - T_i)/(\Delta x/2) \qquad (9b)$$

$$I_{i+\Delta x} = k\,(T_i - T_{i+\Delta x})/(\Delta x/2) \qquad (9c)$$

Eq. (8) may be written as Kirchhoff´s law for the following currents: $I_{i,c} - I_{i-\Delta x} + I_{i+\Delta x} = 0$. The network model for the cell is now designed, Fig. 2a. Eq. (9a) defines a capacitor, C, of variable capacitance (an auxiliary circuit $E_{i,c}$ provides the values of $\mathbf{C}_i(T)$) and eqs. (9b) and (9c) define two resistors of resistance $R_i=\Delta x/2k$. As regards the initial condition, a voltage T_o is applied to the capacitors.

NUMERICAL METHOD

Broadly speaking, the inverse problem, to know the value of the parameters to be estimated in an instant, you must have calculated these parameters in the instant before, is a continual and iterative process composed of two loops, loop approximation (loop internal) and loop stretch (outer loop).

The "loop of stretch" is in charge of taking the whole temperature range and divided it into small sections, to go after scrolling progressively. The data required for this loop are: initial $T(T_{ini})$, final $T(T_{end})$ and number of stretch (Z).

Loop approximation is responsible for running Pspice go with the different values of C, and obtain the optimal $C(C_{opt})$. For each approximation are performed three simulations (C(z), $C(z)+\Delta C$, $C(z)$-ΔC) and take the new value of C that gives smallest error to assign it to C_{opt}. In each new approximation is assigned to $C(z)$ its new value (C_{opt}), as well as reduces the value of $\Delta C_{new}=\Delta C/2$.

The functional to be optimised in each iteration has the classical form

$$F_{(z)} = \Sigma_{(j=n,\, n+1,\, ...,\, n+r)}[T_{inv}(x_f,t_j) - T_{IHCP}(x_f,t_j,\varepsilon_j)]^2 \qquad (10)$$

where z = 1, 2, ... , Z identifies the stretch, Z being the total number of stretches of the piece-wise function. r, which may vary from one stretch to another, is the number of terms of the functional (number of temperature measurements within the actual stretch) and n and n+r are the first and the last temperature index within the stretch, respectively. $T_{inv}(x_f, t_j)$ is the temperature solution of the inverse problem at the position x_f and time t_j. The temperatures $T_{IHCP}(x_f, t_j,\varepsilon_j)$ were defined in the section mathematical model.

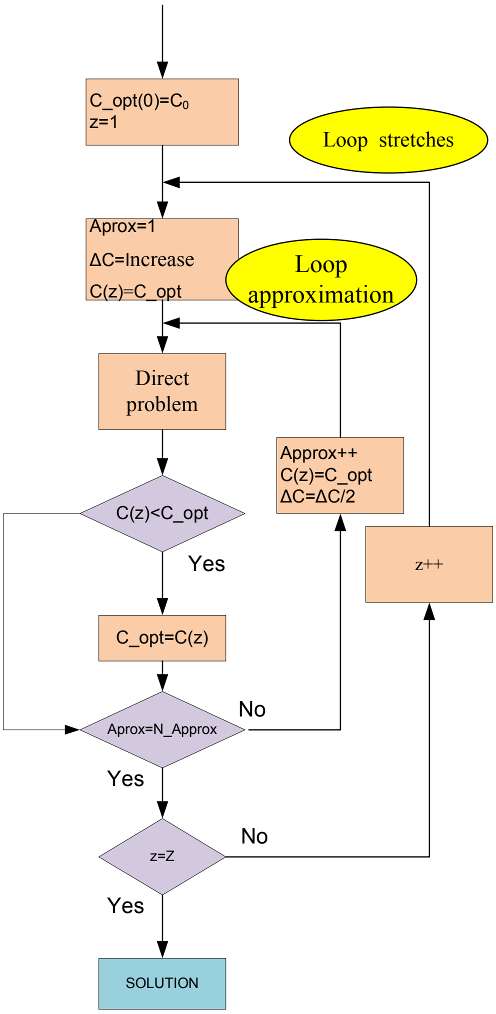

Figure 1 Inverse algorithm of resolution

Software developed

The program consists of three main windows on the first, “Initialization”, we enter the material data. In the second, “Setup” is where you define the type of problem and all the data required for execution. Finally, the third window, "Solution” is showing results.

In the first we met (Figure 2) is the screen charge of the definition of material as well as various properties:

1) Length of body to be treated, measured in meters.

2) Density of the body to be treated, measured in kg/m^3.

3) Initial temperature before of the experiment in ° C.

4) Boundary conditions at the left and right side of the body.
   a. Heat flux measured in W/m^2.
   b. Temperature measured in °C.
   c. Forced convection: Ambient temperature (ºC) and convection coefficient (W/m^2 ºC).

5) Numbers of sensors.

6) Sensor location from the left end in meters.

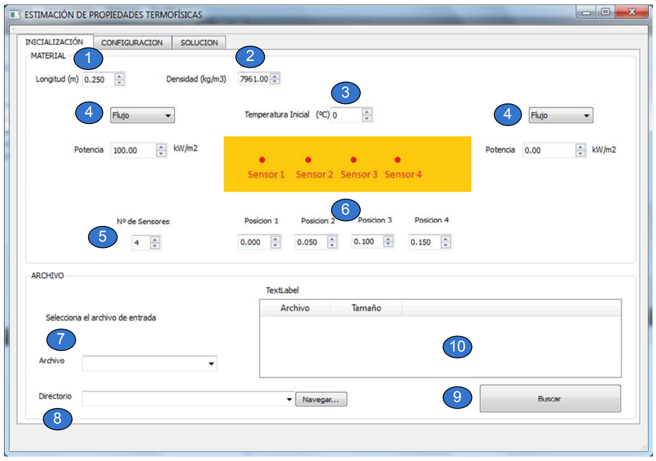

Figure 2 Points of measurement, boundary conditions, ….

Other data (File): It´s necessary only for cases in which wants to solve the inverse problem or the problem of initial value.

7) Name of data file. You must be a plain text file, containing as many columns as the number of sensors for the first time, although it doesn´t affect in the process, its value is purely explanatory. Have no blank line, the first line coincides with the first measurement. You can use asterisks as wildcards.

8) Bar directory where the browser will look for the file specified in paragraph previous.

9) Button to begin your search.

10) Window showing all files in the directory specified and that match the name given in the sections previous. Once displayed, double click on the file to be opened to check the validity of same after verification is already closed and selected.

The “Setup” windows (Figure 3) consists of a series of boxes and buttons that are activated according to the different options we have selected. We can choose between direct problem, the initial value problem and inverse problem. So we can estimate both the thermal conductivity and the specific heat, or both at once. To define the known variables, the program gives us a choice between two options, linear, where we give the initial and final values of the known variables, or stretches, where we can define up to nine stages.

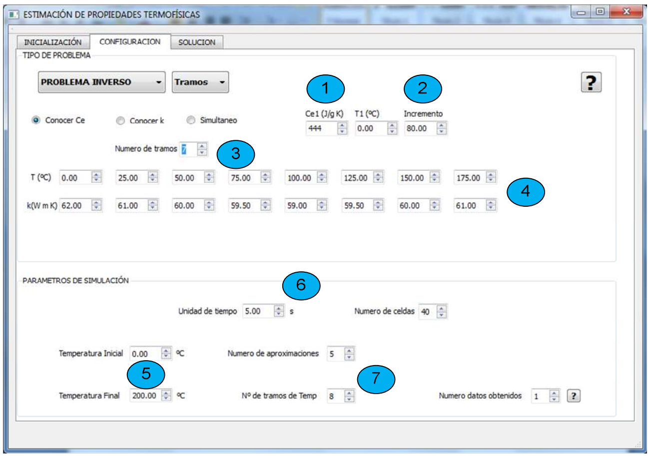

Figure 3 Simulation parameters, stretches, ….

1) Initial value of $C(T)$.

2) ΔC_0 (initial increment heat capacity).

3) Numbers of sections selector to define the specific heat.

4) Table to define the specific heat as a function of temperature.

5) Initial $T(T_{ini})$ and final $T(T_{end})$.

6) Simulation step, must be the same as the input.

7) Numbers of stretches (Z).

In "Solution" window (see Fig. 4), is running the problem chosen and at the end, we show the different simulations. Placing the mouse over the graph, automatically appear calculates parameter values.

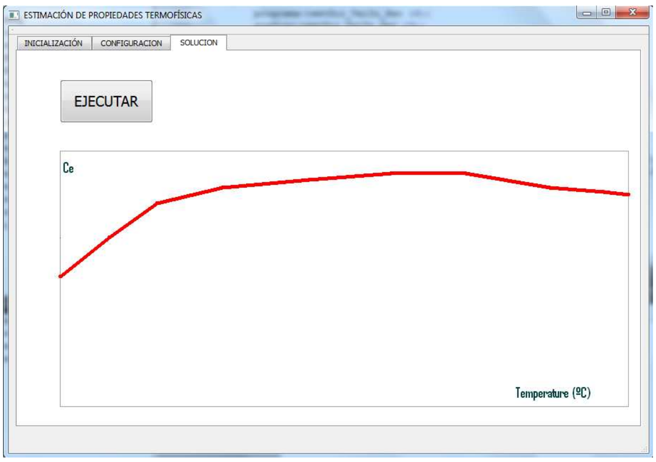

Figure 1 Numerical solution

PROCESSING OF RESULTS

EXPERIMENT 1

First experiment is to know how it affects the error in measuring the position of the sensors in the calculation of the functional. To do this we modeled by a block MESIR tungsten steel L = 250 mm, which is applied at one end a known flow. Measured T(t) at four different points located along the block. Measured were realized from where the flow is applied to the other extreme, so the sensors are placed at x_1 = 0, x_2 = 50 mm, x_3 = 100 mm and x_4 = 150 mm.

Table 1 Results of the experiment 1for a position sensor 1 (x=0)

Position Sensor 1 (mm)	Position Sensor 2 (mm)	Position Sensor 3 (mm)	Position Sensor 4 (mm)	Functional
0	***0.05***	***0.1***	***0.15***	***78.233***
0	0.05	0.1	0.152	346.296
0	0.05	0.1	0.148	412.98
0	0.05	0.102	0.15	657.986
0	0.05	0.102	0.152	926.759
0	0.05	0.102	0.148	992.773
0	0.05	0.098	0.15	710.948
0	0.05	0.098	0.152	979.642
0	0.05	0.098	0.148	1045.685
0	0.052	0.1	0.15	1116.061
0	0.052	0.1	0.152	1383.784
0	0.052	0.1	0.148	1450.678
0	0.052	0.102	0.15	1693.904
0	0.052	0.102	0.152	1961.588
0	0.052	0.102	0.148	2028.501
0	0.052	0.098	0.15	1742.781
0	0.052	0.098	0.152	2018.882
0	0.052	0.098	0.148	2077.527
0	0.048	0.1	0.15	1149.81
0	0.048	0.1	0.152	1450.03
0	0.048	0.1	0.148	1483.231
0	0.048	0.102	0.15	1746.595
0	0.048	0.102	0.152	2046.414
0	0.048	0.102	0.148	2081.046
0	0.048	0.098	0.15	1780.965
0	0.048	0.098	0.152	2081.434
0	0.048	0.098	0.148	2115.326

For discretization we have used 125 cells, so that the size of each cell is Δx =2 mm (L/N). Then calculate functional (we can say that is an error of the estimation), with the various algorithms explained above, modifying the position of the sensors in ±2mm (equivalent to a cell). The results obtained are shown in the tables 1 and 2.

Table 2 Results of the experiment 1 for a position sensor 1 ($x \neq 0$)

Position Sensor 1 (mm)	Position Sensor 2 (mm)	Position Sensor 3 (mm)	Position Sensor 4 (mm)	Functional
0.002	0.05	0.1	0.15	5409.444
0.002	0.05	0.1	0.152	5080.507
0.002	0.05	0.1	0.148	5769.201
0.002	0.05	0.102	0.15	4807.38
0.002	0.05	0.102	0.152	4478.442
0.002	0.05	0.102	0.148	5167.136
0.002	0.05	0.098	0.15	6075.718
0.002	0.05	0.098	0.152	5746.781
0.002	0.05	0.098	0.148	6435.475
0.002	0.052	0.1	0.15	4437.754
0.002	0.052	0.1	0.152	4108.816
0.002	0.052	0.1	0.148	4797.51
0.002	0.052	0.102	0.15	3835.69
0.002	0.052	0.102	0.152	3506.752
0.002	0.052	0.102	0.148	4195.446
0.002	0.052	0.098	0.15	5104.028
0.002	0.052	0.098	0.152	4775.09
0.002	0.052	0.098	0.148	5463.784
0.002	0.048	0.1	0.15	6536.22
0.002	0.048	0.1	0.152	6207.283
0.002	0.048	0.1	0.148	6895.977
0.002	0.048	0.102	0.15	5934.156
0.002	0.048	0.102	0.152	5605.219
0.002	0.048	0.102	0.148	6293.913
0.002	0.048	0.098	0.15	7202.495
0.002	0.048	0.098	0.152	6873.557
0.002	0.048	0.098	0.148	7562.251

In the first row is shown the original position of the sensors, so for this case there is not error in the position of the sensors, so the value of the functional is minimum.

If we compare the first data table with the second, we can see that in the second table the value of the functional is much greater than the first. The error is significantly increased in the second table even though the only difference is the introduction of error in the sensor 1. Likewise if we take the functional groups of five (5 th column, row 1, 2, 3 ...), we see in both tables, the error in the third row is always greater than the error in the second. From these data it appears that the more sensitive functional greater the proximity to the end of the bar (3 rd row). In conclusion we can say that the error in the position of the sensors, affecting directly proportional to the functional, the closer you are the sensors of the constant heat flux applied at x=0.

EXPERIMENT 2

For the next experiment, we take as reference a block of copper cylinder 200mm long and 10mm in diameter (where the mathematical model is the same that for the cartesian coordinate system, due to the problem is one-dimensional), with a density of 1833 kg/m^3 and four k-type thermocouples placed at the positions x =0 mm, x =10 mm, x =20 mm and x=30 mm. It´s applied a constant heat flux of 12.7 W/cm^2 at x=0 where a sensor is located.

Simulating the experiment and obtaining the output temperature sensors, we apply our algorithm of resolution modifying two parameters. On the one hand the number of stretches Z= 10, 20 and 30. To maintain the same range of application of the algorithm, this parameter has to affect inversely proportional to ΔC_0 (see the sensibility equations 11a and 11b)

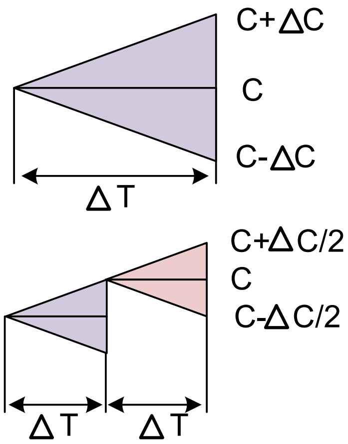

Figure 5 Clarification of the use of ΔC and ΔT

$$Sen = \left(\frac{\Delta C_0}{2^{n^o Aprox}} \right) \cdot Z \qquad (11a)$$

$$Sen' = \left(\frac{\Delta C_0 / (Z'/Z)}{2^{n^o Aprox}} \right) \cdot Z' \overset{z'=2Z}{\Rightarrow} \left(\frac{\Delta C_0 / 2}{2^{n^o Aprox}} \right) \cdot 2Z \qquad (11b)$$

On the other hand it has been changing the value of ΔC_0 following what has been said.

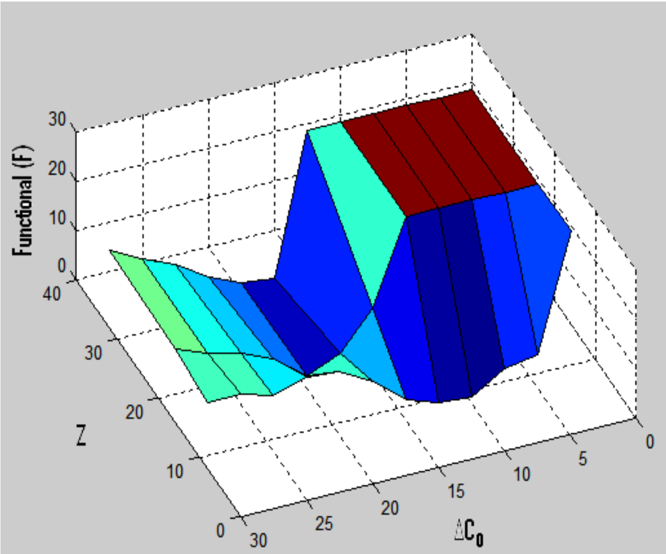

Figure 6 Numerical solution for various values of ΔC and *Z* (experiment 2)

The value of the functional is an appreciation of the error obtained in the estimation of the specific heat (or heat capacity). This value is shown in figure 6 for different values of Z (in the range 5-35) and ΔC_0 (in the range 2.5-30). Minimum value of the functional is obtained for *Z*=10 and ΔC_0=10J/kgK. Figure 7 shows the optimal inverse solution (lowest value of the functional) for the cases, real, *Z*=8 and *Z*=16. We can observed that the better estimation is for *Z*=8 and an instability occurs for *Z*=16.

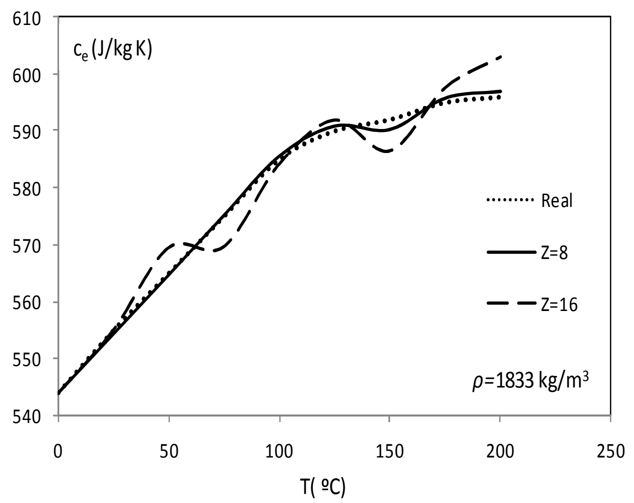

Figure 7 IHCP solution for of $\Delta C_{e,0}$ = 10 J/kgK, for *Z*=8 and 16 (experiment 2)

CONCLUSIONS

This paper provides an efficient numerical software based in the Network Simulation Method already checked in many non-lineal problems) as the numerical tool, for estimating the heat capacity of solid metallic, as a function of the temperature, starting from temperature measurements in a heating process. The proposed procedure is a modification of the known function estimation technique, typical of the inverse problem field. Estimations require various points of measurement in the material.

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