

RESOLUTION OF AN INVERSE PROBLEM FOR IDENTIFICATION OF THERMOPHYSICAL PROPERTIES OF SUBSTANCES TYPICAL OF THE BIOFUELS INDUSTRY

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Abstract. The aim of this work is the estimation of thermal conductivity and specific heat of biofuels in the liquid state. First, was used the finite difference method for the solution of the direct model. Then, was made a sensitivity analysis of the unknown thermophysical properties. Finally, these properties were identified simultaneously by using Levenberg-Marquardt's method. The results present a relative error lower than 0.4% with respect to the exact values of the required parameters.

Keywords: inverse problem, parameter estimation, thermophysical properties, Levenberg-Marquardt's method, biofuel

1. INTRODUCTION

Within the biofuels industry there is a constant concern with regard to the correct sizing of the equipment used during the extraction process, transport and processing of the raw material for biofuels. Engineers has worked in the development and resolution of complex mathematical models in order to predict the thermal properties and dynamic behavior of substances in these industries.

This work presents a stage of the development of an experimental device that can simultaneously identify the thermal properties of substances typical of the biofuels industry. In this paper soya oil and biodiesel were selected as samples. The properties considered are thermal conductivity and specific heat. These properties are estimated by using the Levenberg-Marquardt's method (Beck and Arnold, 1977; Özisik and Orlande, 2000). This technique is a modification of the Gauss method.

Here, the experimental set-up is numerically simulated in order to obtain the transient measurements of temperature in the samples. The values of these temperatures are obtained from boundary conditions and from the direct model solution. This direct model is solved using the finite difference method (Özisik, 1994). The Levenberg-Marquardt's method use the direct model to identify the unknown thermophysical properties of the sample.

2. EXPERIMENTAL SET-UP MODELING

The experimental device is schematized in Fig. 1. It is formed by two cylindrical metallic blocks (A and C). The block-A has thickness L_A and the block-C has thickness L_C . Between these blocks have a cavity of thickness L_B where is stored the substance in liquid state. The device is laterally isolated but some heat is lost through the insulation to the environment (*third kind* boundary condition).

The temperatures at the limits of the two blocks are controlled by heat exchanges, represented by *third kind* boundary condition ($T_{\infty,1}(t)$, h_1 and $T_{\infty,2}(t)$, h_2) in the Fig. 1. The temperature $T_{\infty,1}$ is always higher than $T_{\infty,2}$ and the device is assembled vertically in order to avoid natural convection in the sample. These temperatures are transient, i.e., $T_{\infty,1}(t)$ and $T_{\infty,2}(t)$, where t is the time.

We assume that the sample is homogeneous and opaque. For the two metallic blocks, the thermophysical properties are supposed known and constants with respect to the temperature. One-dimensional heat transfer occurs in the axis y (Fig. 1). Between the metallic blocks and the sample the thermal contact is assumed to be perfect. It is considered that there is no phase change in the sample. The heat transfer in the metallic blocks and in the sample are described by the general differential equation of heat conduction (Incropera, *et al.*, 2011; Çengel and Ghajar, 2012).

$$k_i \frac{\partial^2 T(t,y)}{\partial y^2} + Q_A = \rho_i c_i \frac{\partial T(t,y)}{\partial t} \quad \text{in } L_A < y < L_B, \text{ for } t > 0 \quad (1)$$

$$-k_i \frac{\partial T(t,y)}{\partial y} \Big|_{y=0} = h_1 [T_{\infty,1} - T(t,0)] \text{ in } y=0, \text{ for } t > 0 \quad (2)$$

$$-k_i \frac{\partial T(t,y)}{\partial y} \Big|_{y=L_A} = -k_f \frac{\partial T(t,y)}{\partial y} \Big|_{y=L_A} \text{ in } y=L_A, \text{ for } t > 0 \quad (3)$$

$$\frac{\partial T(t,y)}{\partial y} \left(k_f \frac{\partial T(t,y)}{\partial y} \right) + Q_B = \rho_f c_f \frac{\partial T(t,y)}{\partial t} \text{ in } L_A < y < L_B, \text{ for } t > 0 \quad (4)$$

$$-k_f \frac{\partial T(t,y)}{\partial y} \Big|_{y=L_A+L_B} = -k_i \frac{\partial T(t,y)}{\partial y} \Big|_{y=L_A+L_B} \text{ in } y=L_A+L_B, \text{ for } t > 0 \quad (5)$$

$$k_i \frac{\partial^2 T(t,y)}{\partial y^2} + Q_C = \rho_i c_i \frac{\partial T(t,y)}{\partial t} \text{ in } L_A+L_B < y < L_A+L_B+L_C, \text{ for } t > 0 \quad (6)$$

$$-k_i \frac{\partial T(t,y)}{\partial y} \Big|_{y=L_A+L_B+L_C} = h_2 [T(t,0) - T_{\infty,2}] \text{ in } y=L_A+L_B+L_C, \text{ for } t > 0 \quad (7)$$

$$T(0,y) = T_{ini} \text{ in } 0 < y < L_A+L_B+L_C, \text{ for } t = 0 \quad (8)$$

where k_i is the thermal conductivity of the block-A and block-C, k_f is the thermal conductivity of the sample. The specific heat of the metallic blocks is defined by c_i and for the sample by c_f . The parameter ρ_i is the density of the block-A and block-C, ρ_f is the density of the sample. The heat transfer coefficient at the top, the bottom and the side of the device are given by h_1 , h_2 and h_e , respectively. The temperature T_{∞} is the external temperature of the device. The variables Q_A , Q_B and Q_C are the heat losses in the block-A, sample and block-C, respectively.

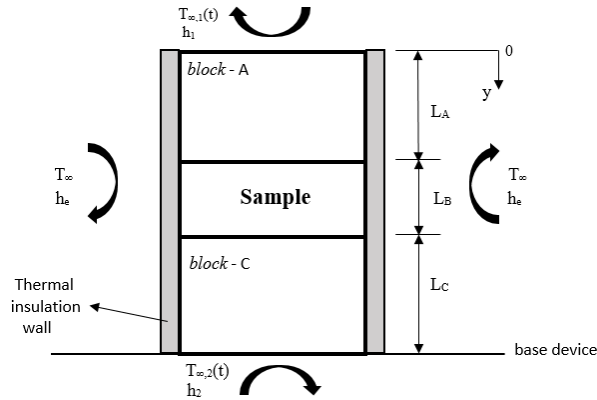


Figure 1. Experimental set-up

The transient measurements of temperature are obtained for three temperature sensors in three different positions at the sample. Those positions are shown in Fig. 2, where S1 is the sensor 1, S2 is the sensor 2 and S3 is the sensor 3.

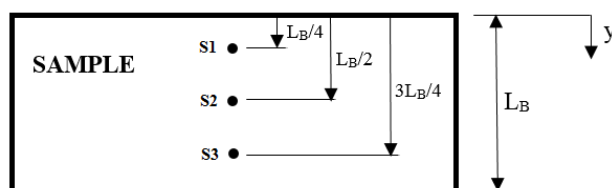


Figure 2. Positions of the temperature sensors at the sample.

3. DIRECT MODEL

The finite difference method (Özisik, 1994) was used to solve the Eq. (1) to Eq. (8). In this numerical technique, the domain is discretized at a finite number of nodal points. We used the explicit form of finite difference approximation that the unknown nodal temperatures T_m^{p+1} for the time level $p+1$ are calculated from known nodal temperatures in the previous time level p .

The block-A is divided in m_A nodes, $1 \leq m_A \leq N_A$, where N_A is the total number of nodes in the block-A. The sample is divided in m_B nodes, $N_A + 1 \leq m_B \leq N_A + N_B - 1$, where N_B is the total number of nodes in the sample. The block-C is divided in m_C nodes, $N_A + N_B \leq m_C \leq N_A + N_B + N_C - 2$, where N_C is the total number of nodes in the block-C.

$$T_{m_A}^{p+1} = \frac{2h_1\Delta t}{\rho_i c_i \Delta y_A} T_{\infty,1}(t) + \left(1 - \frac{2h_1\Delta t}{\rho_i c_i \Delta y_A} - \frac{2k_i\Delta t}{\rho_i c_i \Delta y_A^2} - \frac{h_e\Delta t}{\rho_i c_i \Delta y_A} \right) T_{m_A}^p + \frac{2k_i\Delta t}{\rho_i c_{pi} \Delta y_A} T_{m_A+1}^p + \frac{h_e\Delta t}{\rho c_p \Delta y_A} T_{\infty} \text{ in } m_A=1 \quad (9)$$

$$T_{m_A}^{p+1} = \frac{k_i\Delta t}{\rho_i c_i \Delta y_A^2} T_{m_A-1}^p + \left(1 - \frac{2k_i\Delta t}{\rho_i c_i \Delta y_A^2} - \frac{h_e\Delta t}{\rho_i c_i \Delta y_A} \right) T_{m_A}^p + \frac{k_i\Delta t}{\rho_i c_i \Delta y_A^2} T_{m_A+1}^p + \frac{h_e\Delta t}{\rho_i c_i \Delta y_A} T_{\infty} \text{ in } 2 < m_A < N_A \quad (10)$$

$$T_{m_A}^{p+1} = \frac{2k_i\Delta t}{\rho_i c_i (\Delta y_A + \Delta y_B) \Delta y_A} T_{m_A-1}^p + \left\{ 1 - \frac{2k_i\Delta t}{\rho_i c_i (\Delta y_A + \Delta y_B) \Delta y_A} - \frac{2k_f\Delta t}{\rho_f c_f (\Delta y_A + \Delta y_B) \Delta y_B} - \frac{h_e\Delta t}{(\Delta y_A + \Delta y_B) \left[\frac{1}{\rho_i c_i} + \frac{1}{\rho_f c_f} \right]} \right\} T_{m_A}^p + \frac{2k_f\Delta t}{\rho_f c_f (\Delta y_A + \Delta y_B) \Delta y_B} T_{m_A+1}^p + \frac{h_e\Delta t}{(\Delta y_A + \Delta y_B) \left[\frac{1}{\rho_i c_i} + \frac{1}{\rho_f c_f} \right]} T_{\infty} \text{ in } m_A = N_A \quad (11)$$

$$T_{m_B}^{p+1} = \frac{k_f\Delta t}{\rho_f c_f \Delta y_B^2} T_{m_B-1}^p + \left(1 - \frac{2k_f\Delta t}{\rho_f c_f \Delta y_B^2} - \frac{h_e\Delta t}{\rho_f c_f \Delta y_B} \right) T_{m_B}^p + \frac{k_f\Delta t}{\rho_f c_f \Delta y_B^2} T_{m_B+1}^p + \frac{h_e\Delta t}{\rho_f c_f \Delta y_B} T_{\infty} \text{ in } N_A + 1 \leq m_B \leq N_A + N_B - 2 \quad (12)$$

$$T_{m_B}^{p+1} = \frac{2k_f\Delta t}{\rho_f c_f (\Delta y_B + \Delta y_C) \Delta y_B} T_{m_B-1}^p + \left\{ 1 - \frac{2k_i\Delta t}{\rho_i c_i (\Delta y_B + \Delta y_C) \Delta y_C} - \frac{2k_f\Delta t}{\rho_f c_f (\Delta y_B + \Delta y_C) \Delta y_B} - \frac{h_e\Delta t}{(\Delta y_B + \Delta y_C) \left[\frac{1}{\rho_i c_i} + \frac{1}{\rho_f c_f} \right]} \right\} T_{m_B}^p + \frac{2k_i\Delta t}{\rho_i c_i (\Delta y_B + \Delta y_C) \Delta y_C} T_{m_B+1}^p + \frac{h_e\Delta t}{(\Delta y_B + \Delta y_C) \left[\frac{1}{\rho_i c_i} + \frac{1}{\rho_f c_f} \right]} T_{\infty} \text{ in } m_B = N_A + N_B - 1 \quad (13)$$

$$T_{m_C}^{p+1} = \frac{k_i\Delta t}{\rho_i c_i \Delta y_C^2} T_{m_C-1}^p + \left(1 - \frac{2k_i\Delta t}{\rho_i c_i \Delta y_C^2} - \frac{h_e\Delta t}{\rho_i c_i \Delta y_C} \right) T_{m_C}^p + \frac{k_i\Delta t}{\rho_i c_i \Delta y_C^2} T_{m_C+1}^p + \frac{h_e\Delta t}{\rho_i c_i \Delta y_C} T_{\infty} \text{ in } N_A + N_B \leq m_C \leq N_A + N_B + N_C - 3 \quad (14)$$

$$T_{m_C}^{p+1} = \frac{2h_2\Delta t}{\rho_i c_i \Delta y_C} T_{\infty,2}(t) + \left(1 - \frac{2h_2\Delta t}{\rho_i c_i \Delta y_C} - \frac{2k_i\Delta t}{\rho_i c_i \Delta y_C^2} - \frac{h_e\Delta t}{\rho_i c_i \Delta y_C} \right) T_{m_C}^p + \frac{2k_i\Delta t}{\rho_i c_i \Delta y_C^2} T_{m_C+1}^p + \frac{h_e\Delta t}{\rho_i c_i \Delta y_C} T_{\infty} \text{ in } m_C = N_A + N_B + N_C - 2 \quad (15)$$

The parameters Δy_A , Δy_B and Δy_C are the distance between each node in the block-A, the sample and the block-C, respectively. The time step is indicated by Δt . The explicit method imposes a limit for the value of the time step. In this case, Δt is determined by stability criterion (Özisik, 1994) given by:

$$\Delta t \leq \frac{\rho_i c_i \Delta y}{2h + \frac{2k_i}{\Delta y} + h_e} \quad (16)$$

4. VERIFICATION OF THE DIRECT MODEL

The numerical solution of the model is calculated using MATLAB software and then this solution is compared with the simulation in ANSYS software. The thermal properties (thermal conductivity and specific heat) used for the simulation are taken from soya oil (Brock, *et al.*, 2008; Nouredini, *et al.*, 1992; Santos, *et al.*, 2005).

Figure 3 shows the temperature-time variation for three points inside the sample. These points are shown in Fig. 2. The maximum relative errors found are smaller than 0.5%.

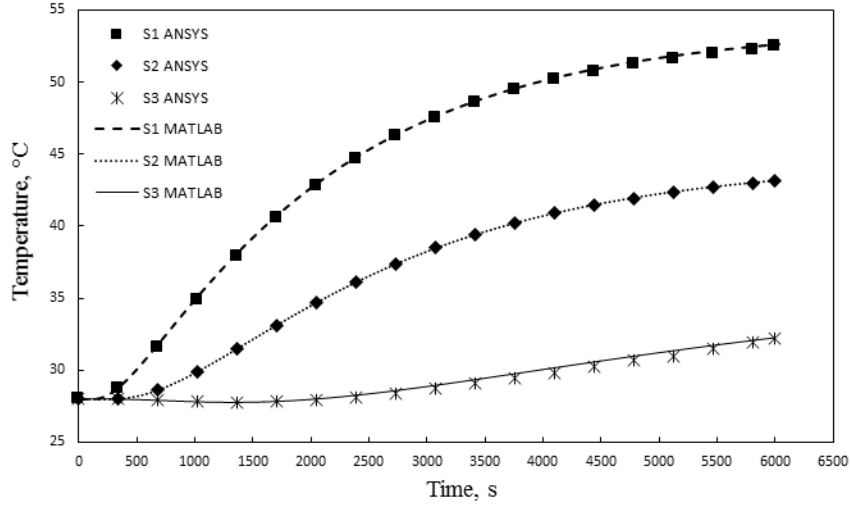


Figure 3. Numerical validation

5. PARAMETER ESTIMATION

According to Özisik and Orlande (2000), the parameter estimation problem is solved by minimizing the least-squares norm (sum of the squared residuals) with respect to the unknown parameters. This norm is called objective function, $S(\mathbf{P}, t)$. The objective function written in matrix form as:

$$S(\mathbf{P}) = [\mathbf{Y}(t) - \mathbf{T}(\mathbf{P}, t)]^T \cdot [\mathbf{Y}(t) - \mathbf{T}(\mathbf{P}, t)] \quad (17)$$

where $\mathbf{P}$ is a vector that contains the parameters to be estimated; $\mathbf{Y}$ is the matrix of the measured temperatures, Eq. (19) at time t ; and $\mathbf{T}$ is the matrix of estimated temperatures, Eq. (20), which is a function of $\mathbf{P}$ and t . The superscript T indicates the transpose.

The vector $\mathbf{P}$ is defined as:

$$\mathbf{P} = [k, c_p] \quad (18)$$

The measured temperatures, $\mathbf{Y}$, are obtained by numerical simulation of the experimental set-up. This solution provides the transient temperatures measurements in three points at the sample as shown in Fig. 2. So:

$$\mathbf{Y} = [T_1(t), T_2(t), T_3(t)] \quad (19)$$

By the direct model (Eq. 9-15) we obtain the values of $\mathbf{T}$:

$$\mathbf{T} = [T_{1e}(t), T_{2e}(t), T_{3e}(t)] \quad (20)$$

The Levenberg-Marquardt's method (Beck and Arnold, 1977; Özisik and Orlande, 2000) is used to optimize the values of the vector $\mathbf{P}$ so as to minimize the objective function $S(\mathbf{P}, t)$. The interactive procedure is given by:

$$\mathbf{P}^{w+1} = \mathbf{P}^w + [(J(\mathbf{P})^w)^T \cdot J(\mathbf{P})^w + \mu^w \cdot \mathbf{\Omega}^w]^{-1} \cdot (J(\mathbf{P})^w)^T \cdot [\mathbf{Y} - \mathbf{T}(\mathbf{P}^w)] \quad (21)$$

where the superscript w denotes the number of iterations, μ is a damping parameter and $\mathbf{\Omega}$ is a diagonal matrix defined as:

$$\mathbf{\Omega}^w = \text{diag}[(J(\mathbf{P})^w)^T \cdot J(\mathbf{P})^w] \quad (22)$$

where $J(\mathbf{P})$ is the sensitivity matrix or Jacobian matrix:

$$J(\mathbf{P}) = \left[\frac{\partial \mathbf{T}^T(\mathbf{P}, t)}{\partial \mathbf{P}} \right]^T \quad (23)$$

and its reduced form is:

$$J^*(P) = P.J(P) \quad (24)$$

The elements of the sensitivity matrix are called sensitivity coefficients. Thanks to the sensitivity coefficients analysis, the Levenberg-Marquardt's algorithm can be optimized (Beck and Arnold, 1977; Özisik and Orlande, 2000). The identification iterative methodology used is resumed in the following basic steps:

Step 1. Compute $S(P^w)$ from Eq. (17), by using the initial values adopted to the vector P^w , Eq. (18).

Step 2. Compute J^w , Eq. (23), and then the matrix Ω^w , Eq. (22).

Step 3. Solve the linear system of algebraic equations obtained from the interactive procedure of the Levenberg-Marquardt's method, Eq. (21), in order to find P^{w+1} .

Step 4. Solve the direct problem, Eq. (9) to Eq. (15), with P^{w+1} in order to find $T(P^{w+1})$. Then calculate $S(P^{w+1})$.

Step 5. If $S(P^{w+1}) \geq S(P^w)$, replace μ^w by $10\mu^w$ and return to step 3. If $S(P^{w+1}) < S(P^w)$, accept the P^{w+1} and replace μ^w by $0.1\mu^w$.

Step 6. Check the stopping criteria given by Eq. (25).

$$S(P^{w+1}) < \varepsilon \quad (25)$$

where ε is the tolerance value (here, $\varepsilon \approx 1e-2$).

6. SENSITIVITY COEFFICIENT ANALYSIS

The analysis of the sensitivity coefficients is an important part of all the inverse problems of parameter estimation. There are some direct models for which it is not possible to estimate simultaneously all unknown parameters in a single experiment (Liu and Han, 2003; Özisik and Orlande, 2000; Beck and Arnold, 1977). The sensitivity analysis allowed to highlight the influence of the parameters k and c_p (Eq. 18) on the calculated temperatures T (Eq. 20) by the direct model and check the possibility that these two parameters be estimated simultaneously.

The soya oil was chose as material-test with the followings parameters (Brock, *et al.*, 2008; Nouredini, *et al.*, 1992; Santos, *et al.*, 2005): $k = 0.1693 \text{ W.m}^{-1}.\text{K}^{-1}$ and $c_p = 2591 \text{ J.kg}^{-1}.\text{K}^{-1}$.

The experimental methodology is as followed: at the beginning, the temperature in the two metallic blocks and the sample is uniform. Then, the temperatures $T_{\infty,1}(t)$ and $T_{\infty,2}(t)$ are decreased simultaneously and after this, these temperatures are increased until to return the initial temperature.

Each column of the sensitivity matrix is plotted as shown Fig. 4, 5 and 6.

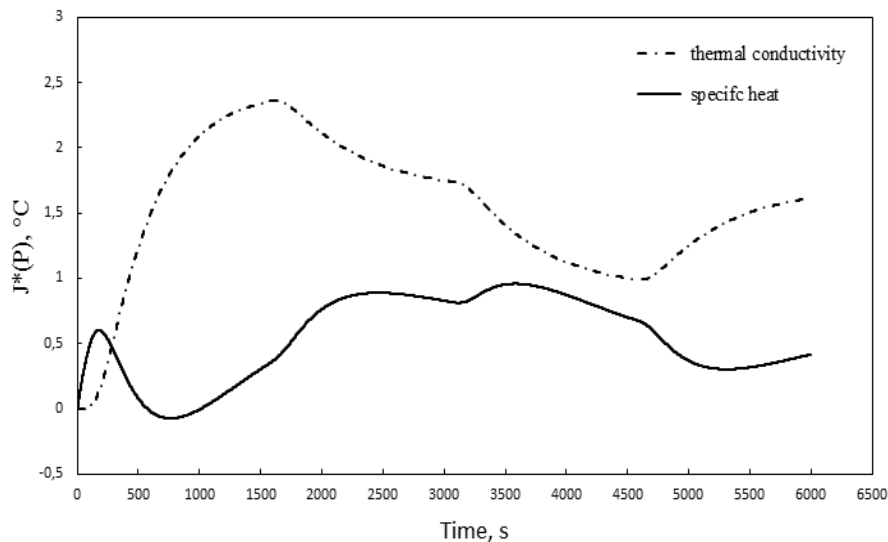


Figure 4. Sensitivity coefficients at sensor 1

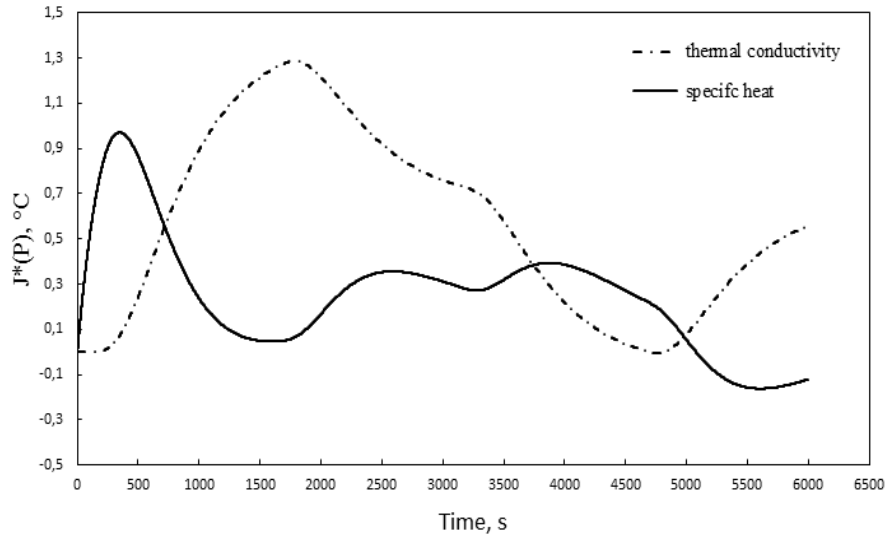


Figure 5. Sensitivity coefficients at sensor 2

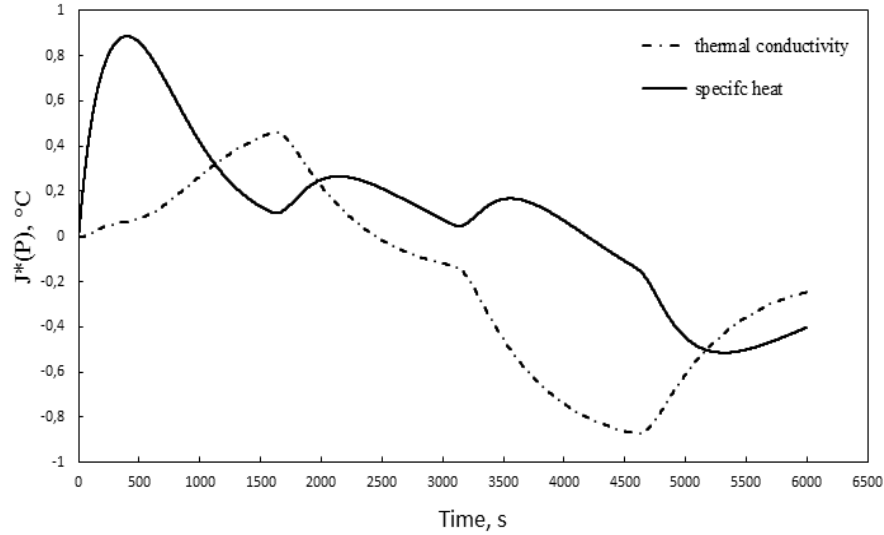


Figure 6. Sensitivity coefficients at sensor 3

From Fig. 4, 5 and 6 it can be noted that the parameters k and c_p can be simultaneously estimated because they are not linearly dependent. Another method is used to know if these parameters are linearly dependent. It is called *identifiability condition* (Özisik and Orlande, 2000). If the determinant of $J^T J$ is zero, or even very small, the parameters cannot be simultaneously determined by using the interactive procedure of Eq. (21).

$$\theta = \det[J(P)^T J(P)] \quad (26)$$

Using the Eq. (26), $\theta = 2.0068e3$. This result indicates that the parameters k and c_p can be simultaneously estimated.

7. RESULTS AND DISCUSSION

For the first test-case, the k and c_p of the soya oil and biodiesel was estimated considering the absence of noise in the measured temperatures, Y (Eq.19). The initial guesses of the parameters were taken distant 50% approximately of the literature data (Brock, *et al.*, 2008; Nouredini, *et al.*, 1992; Santos, *et al.*, 2005; Methanol Institute, 2011). The maximal relative error found was smaller than 0.4%, Tab. 1 and Tab. 2. For the case of soya oil five iterations was necessary ($w = 5$) while for the biodiesel $w = 7$.

Table 1. Estimated parameters of soya oil

	k $W.m^{-1}.K^{-1}$	c_p $J.kg^{-1}.K^{-1}$
Real data	0.1693	2591
Initial values	0.2540	3886
Iteration, $w = 1$	0.1651	2639
Iteration, $w = 3$	0.1686	2618
Iteration, $w = 5$ (estimated)	0.1691	2600
Relative error (%)	0.12	0.35
Confidence interval	± 0.000	± 1.207

Table 2. Estimated parameters of biodiesel

	k $W.m^{-1}.K^{-1}$	c_p $J.kg^{-1}.K^{-1}$
Real data	0.1730	1800
Initial values	0.2600	2700
Iteration, $w = 1$	0.1528	2270
Iteration, $w = 3$	0.1684	1912
Iteration, $w = 7$ (estimated)	0.1728	1806
Relative error (%)	0.11	0.33
Confidence interval	± 0.000	± 1.125

For the second test-case, the k and c_p of the soya oil and biodiesel was estimated considering *Gaussian noise* (Mathuranathan, 2013) in the measured temperatures, Y (Eq.19). The standard deviation chosen was $\sigma = 0.02$ °C, $\sigma = 0.05$ °C and $\sigma = 0.08$ °C. The initial guesses of the parameters were taken distant 50% approximately of the literature data. Similar to the first test-case, the maximal relative error found was smaller than 0.4%, Tab. 3 and Tab. 4. However the number of iteration increased, compared with to the last test-case. For the case of soya oil the maximum number of iterations was $w = 11$ and while for biodiesel $w = 14$.

Table 3. Estimated parameters of soya oil with Gaussian noise.

	k $W.m^{-1}.K^{-1}$	c_p $J.kg^{-1}.K^{-1}$
Real data	0.1693	2591
Initial values	0.2540	3886
$\sigma = 0.02$		
Number of Iterations	11	11
Value estimated	0.1693	2593
Relative error (%)	0.00	0.08
Confidence interval	± 0.000	± 0.943
$\sigma = 0.05$		
Number of Iterations	11	11
Value estimated	0.1691	2601
Relative error (%)	0.12	0.39
Confidence interval	± 0.001	± 1.487
$\sigma = 0.08$		
Number of Iterations	10	10
Value estimated	0.1692	2596
Relative error (%)	0.06	0.19
Confidence interval	± 0.002	± 1.822

Table 4. Estimated parameters of biodiesel with Gaussian noise.

	k $W.m^{-1}.K^{-1}$	c_p $J.kg^{-1}.K^{-1}$
Real data	0.1730	1800
Initial values	0.2600	2700
$\sigma = 0.02$		
Number of Iterations	14	14
Value estimated	0.1728	1805
Relative error (%)	0.11	0.28
Confidence interval	± 0.000	± 1.009
$\sigma = 0.05$		
Number of Iterations	12	12
Value estimated	0.1729	1803
Relative error (%)	0.06	0.17
Confidence interval	± 0.001	± 1.556
$\sigma = 0.08$		
Number of Iterations	14	14
Value estimated	0.1729	1802
Relative error (%)	0.06	0.11
Confidence interval	± 0.003	± 1.911

Confidence intervals (Özisik and Orlande, 2000), shown in tables 1, 2, 3 and 4, are for 99% confidence level.

8. CONCLUSIONS

An inverse problem is solved to estimate the k and c_p of two biofuels samples. The sensitivity analysis provides essential information for the optimization of the estimation algorithm. In fact, this analysis showed that the parameters k and c_p can be simultaneously estimated through Levenberg-Marquardt's method.

The estimation results (obtained from simulated transient measurements of the temperatures) were satisfactory. The tables 1, 2, 3 and 4 show that relative errors between the values of the estimated parameters and the literature data were smaller than 0.4%, even with the introduction of noises in the measured temperatures.

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10. RESPONSABILITY NOTICE

The authors are the only responsible for the printed material included in this paper.