AN INVERSE ANALYSIS FOR SIMULTANEOUS THERMAL PARAMETER ESTIMATION IN ADSORPTIVE POROUS PACKED BEDS

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Abstract. This paper presents an inverse analysis for simultaneous estimation of a boundary condition and effective thermal diffusivity in an adsorptive porous media formed by activated carbon and pure methane gas. These parameters are estimated from the solution of the inverse heat conduction problem, through the attribution of initial values to effective thermal diffusivity and quartic polynomial coefficients which represent the boundary condition of transient temperature. The experimental setup designed to conduct experiments with micro-porous materials in presence of several gases has provided the foundations for the physical modeling of the problem studied. Transient temperature distributions are determined theoretically and by experimental simulation. In the direct analysis, temperature profile of the porous media, under local thermodynamic equilibrium hypothesis, is determined employing Thomas algorithm. Concerning to the inverse analysis, the best combination for effective thermal diffusivity and quartic polynomial coefficients is reached when least-squares errors between theoretical and simulated temperature values are minimized. Here, Levenberg-Marquardt regularization iterative algorithm is applied to solve the non-linear system of algebraic equations resulting from the sensitivity matrix. Results and uncertainties are presented and discussed for effective thermal diffusivity as well as the boundary condition. The influence of measurement errors is also analysed.

***Keywords**: thermal parameters, direct problem, sensitivity analysis, simultaneous estimation and inverse problem.*

1. Introduction

Heat transfer in porous media is characterized by a complex mechanism of conduction, convection and radiation. Assuming that the temperatures of the gas phase and the solid matrix are in local thermodynamic equilibrium, both phases can be treated as a simple artificial one. Therefore only one parameter – the effective thermal conductivity – is necessary as it cumulates conduction, convection and radiation effects.

Several theoretical and experimental methods are explained in the literature to estimate materials thermophysical properties. Concerning to porous media, investigations about thermal conductivity are predominant. In these studies, thermophysical properties depend on thermal characteristics of the adsorbing solid and the adsorbed phase, the contact geometry between particles and the bed porosity. There have been models for calculation of thermal conductivity of packed beds and powdered insulations, notable among them are those described by Kunii and Smith (1960), Luikov *et al*. (1968) and Bauer and Schlünder (1978). These models assume that there is no gaseous adsorption by the solid particles. Tsotsas and Martin (1987) present a review of investigations involving thermal conductivity of packed beds. In recent studies, Gurgel and Grenier (1990) determined the effective thermal conductivity of a granular packed bed composed by activated carbon in presence of different gases. Prakash *et al.* (2000) proposed an empirical correlation based on the model developed by Luikov *et al*. (1968) to describe the dependence of effective thermal conductivity on the packing density and temperature. This model is utilized by Basumatary *et al*. (2005) to proceed to the thermal modeling of an activated carbon based adsorptive natural gas storage system.

The interest of inverse heat conduction problems relies on the identification of thermophysical properties and/or boundary conditions of a system where direct measurements are impracticable, through the use of remote temperature measurements taken either within the system itself or on a different part of the surface (Prud'homme and Nguyen, 2001). This specific problem is of interest in a large range of scientific and engineering areas including manufacturing processes control, metallurgy, chemistry, aerospace and nuclear engineering, food science, medical diagnosis, etc.

A large amount of information is available in the literature regarding inverse conduction problems encountered in the design, control and identification of thermal systems. Much less information can be found on inverse problem involving porous media. This is specifically true concerning to the identification of effective thermal diffusivity in adsorptive porous packed beds, where empirical models for effective thermal conductivity estimation predominate.

This paper studies an inverse heat conduction problem for simultaneous estimation of boundary condition and effective thermal diffusivity in an adsorptive packed bed constituted by activated carbon and pure methane gas. An experimental apparatus has provided the foundations for the physical modeling of the problem. The solution of the problem is based on thermal parameter estimation attached to the combination of theoretical results, obtained from the direct problem solution, and numerical simulations, which are presented and discussed. Solving this inverse problem is important for heat transfer processes evaluations considered in the designing and sizing of automotive tanks for natural gas storage through adsorption on activated carbon packed beds. Since natural gas primarily consists of methane, it is idealized here as pure methane for calculation purposes. Methane adsorption on activated carbon is an exothermic process and the heat of adsorption generated influences directly the ability of the bed to store natural gas.

2. Experimental setup description

The experimental apparatus here presented has the aim to allow the measurement of temperature transient profiles in a porous media bed at a time interval Δt. This experimental setup, proposed from Tsotsas and Martin (1987) studies, is successfully used by Pereira *et al.* (1991) and also Gurgel and Grenier (1990). Experiments with similar configurations have been conducted by Basumatary *et al.* (2005). The simulated experimental results found in this paper are based on the following apparatus description.

The apparatus consists of a vertical cast iron cylindrical reactor whose geometric dimensions are: internal diameter $D_{\text{int}} = 100\,\text{mm}$, height of the bed $H_b = 250\,\text{mm}$ and cylinder height $H_c = 350\,\text{mm}$. The sample of material test is packed as a pallet bed, limited in the upper and lower ends by stainless steel discs. A Ni-Cr electrical resistance wire, 0,198 mm diameter, is placed axially in the cylinder centre where it dissipates a uniform heat flow in the symmetry axis of the sample, generated from a constant electrical power.

In the central plane of the cylinder, four thermal sensors are distributed radially to register the temperature distribution of the bed during the progress of time. Design distance between the sensors is 10 mm. The thermal sensors utilized in this setup are Pt $100\,\Omega$ resistors. The temperature register is controlled by a digital data acquisition system connected to a microcomputer (Intel Pentium IV processor, 1,5 GHz, RAM memory of 256 MB).

The sealing cover, positioned immediately above the reactor, has three flanged inputs for gas supply, internal pressure control or vacuum monitoring and temperature sensors connection cables. Figure 1 illustrates the given experimental setup description with a schematic diagram and a photograph.

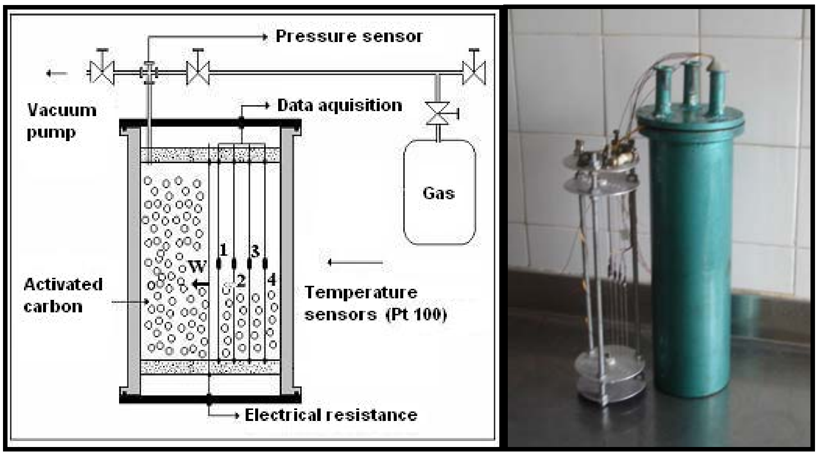

Figure 1. Schematic diagram (left) and photograph (right) of the experimental apparatus

Specifically for this reactor, two-dimensional effects in the central plane of the cylinder are neglected once is satisfied a particular relation, established during the design period, between the height of the bed H_b and the internal diameter of the cylinder D_{int}. In accordance with Gurgel and Klüppel (1996) as also stated by Pereira *et al.* (1991), axial heat losses will have negligible influence $(\varepsilon < 1\%)$ in thermal conductivity measurement accuracy of packed beds whose conductivities exhibit small values $\left(k_b \cong 0,2\ \text{W}/(\text{m}\cdot\text{K})\right)$ whether reactor geometric dimensions satisfy the ratio $H_b / D_{\text{int}} > 2,5$.

The experimental apparatus showed in Fig. 1 is based upon a mathematical model agreeable with a heat diffusion experience in an adsorptive porous media. Temperatures are measured in two distinct locations (thermal sensors 1 and 2) after submitting the bed to a thermal perturbation generated by heat power dissipation. One of the thermograms is used as a boundary condition and the other assists to establish a comparison between these values and those ones obtained from the numerical solution of the heat diffusion problem. Heat flow dissipated by the electrical resistance compounds the final boundary condition. Temperatures obtained in sensors 3 and 4 are not used in this study.

3. Direct problem

Consider a granular porous packed bed constituted by activated carbon and pure methane gas, limited by a cylindrical cavity at a uniform initial temperature $T_{initial}$. At time t, it is heated by an electrical resistance positioned in the centre of the cylindrical cavity which dissipates uniformly a heat flow q'' in the radial direction. It is assumed that the porous media is homogenous, isotropic, no internal heat generation is observed and it is characterized by an effective thermal diffusivity α_{ef}. Let i, $i = 0,1,2$, be an identification index whose terms have the following meaning: (0) – cylindrical cavity centre; (1) – position of the thermal sensor 1 and (2) – position of the thermal sensor 2. Time dependent temperature profile T is obtained from the solution of the one-dimensional heat diffusion equation – Eq. (1) – subjected to the following boundary conditions and initial condition – Eqs. (2 a 4):

$$\frac{\partial^2 T(r,t)}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial T(r,t)}{\partial r} = \frac{1}{\alpha_{ef}} \cdot \frac{\partial T(r,t)}{\partial t}, \text{ for } 0 \le r \le R \tag{1}$$

Boundary conditions:

$$-k_b \cdot \left. \frac{dT}{dr} \right|_{r=r_0} = q'' = \frac{W}{A_l} = \frac{W}{2 \cdot \pi \cdot r_0 \cdot H_b}, \text{ for } r = r_i, \text{ when } i = 0 \tag{2}$$

$$T(r_2, t) = f(t), \text{ for } r = r_i, \text{ when } i = 2 \tag{3}$$

Initial condition:

$$T(r,0) = T_{initial}, \text{ for } 0 \le r \le R \tag{4}$$

where W represents the constant heat power, r is the radial position, k_b is the thermal conductivity of the packed bed and A_l is the lateral surface area of the Ni-Cr wire that dissipates W.

Equations (1) to (4) are solved numerically applying a semi-implicit finite difference method. Control volume approximation is admitted in order to accomplish the correct form of the finite difference equations and Crank-Nicolson technique is employed to determine temperature field in the calculus domain (Özisik, 1994). In addition to the admitted assumptions, it is also considered:

- The solid matrix can be idealized to be undeformable and is in thermal equilibrium with the methane gas;
- Intraparticle and film resistances to heat transfer are negligible;
- Viscosity and specific heat of methane are not temperature dependent;
- Cylindrical cavity is hollowed with internal radius equal to Ni-Cr wire radius, which is, $r_{\text{int}} = r_0 = 0,099$ mm;
- Calculus domain is divided in a mesh composed by $M = 30$ nodal points in radial direction;
- Boundary condition function $f(t)$ in Eq. (3) is admitted to be a quartic polynomial.

The finite difference system of algebraic equations is solved applying Thomas algorithm (Fortuna, 2000). Computational implementation is developed with the Microsoft Fortran Powerstation 4.0 software.

4. Inverse problem

The inverse problem is concerned with the simultaneous estimation of quartic polynomial coefficients $(a_0$, a_1, a_2, a_3 and $a_4)$, which represents a boundary condition in r_2, and effective thermal diffusivity α_{ef} from the measured temperature response at r_1. The experimental conditions are those defined previously and assumed to be well known. The measured temperature data may contain random errors. The problem is to compute the estimates of these parameters which will minimize the least-squares norm between experimental temperature values and theoretical values originated from the equation system already discussed – Eqs. (1 to 4).

Let $\mathbf{T_E}$ and $\mathbf{T}$ be the vectors that represent experimental and theoretical temperature profiles, respectively; and $\boldsymbol{\psi}$ is the covariance matrix of measured errors. The least-squares norm to maximum likelihood estimator $S(\boldsymbol{\beta})$ can be written in matrix form as (Beck and Arnold, 1977):

$$S(\boldsymbol{\beta}) = \left[\mathbf{T_E} - \mathbf{T}(\boldsymbol{\beta})\right]^T \boldsymbol{\psi}^{-1} \left[\mathbf{T_E} - \mathbf{T}(\boldsymbol{\beta})\right] \quad (5)$$

where

$$\left[\mathbf{T_E} - \mathbf{T}(\boldsymbol{\beta})\right]^T = \left[T_E(t_1) - T(t_1;\beta), \ldots, T_E(t_n) - T(t_n;\beta)\right] \quad (6)$$

$$\boldsymbol{\beta}^T = \left[\beta_1, \beta_2, \ldots, \beta_m\right] = \left[a_0, a_1, a_2, a_3, a_4, \alpha_{ef}\right] \text{ , for } m = 1, 2, \ldots, p. \quad (7)$$

$T_E(t_j)$ are the experimental temperatures generated by numerical simulation at time t_j; n is the total number of measurements and p is the number of parameters to determine. The estimated temperatures $T(t_j;\beta)$ at time t_j and at the measurement locations are obtained from the solution of the finite difference system of equations by using the estimation for the unknown vector $\boldsymbol{\beta}$.

As maximum likelihood estimation is the estimation method chosen, the following standard statistical assumptions, listed by Beck and Arnold (1977), are considered: additive errors with zero mean and normal probability distribution; unknown statistical parameters; nonstochastic independent variable; no prior information regarding the parameters to determine and parameters nonrandom.

Due to the considered hypothesis, variable $S(\boldsymbol{\beta})$ in Eq. (5) follows a χ^2 distribution for $v = n - p$ degrees of freedom. Hence, maximum likelihood estimation is performed by the minimization of χ^2 statistic. The probability value calculated for χ^2 indicates a goodness of fit measure (Press *et al.*, 1989). Beck and Arnold (1977) state that the following condition should be satisfied in order to minimize the least-squares norm for the maximum likelihood estimator:

$$\nabla_\beta S(\boldsymbol{\beta}) = 2\left[-\nabla_\beta \mathbf{T}^T(\boldsymbol{\beta})\right] \boldsymbol{\psi}^{-1} \left[\mathbf{T_E} - \mathbf{T}(\boldsymbol{\beta})\right] = 0 \quad (8)$$

Equation (9) gives the term that represents sensitivity matrix (Tang and Araki, 2000):

$$\mathbf{X}(\boldsymbol{\beta}) = \left[\nabla_\beta \mathbf{T}^T(\boldsymbol{\beta})\right]^T = \begin{bmatrix} X_{1a_0} & X_{1a_1} & X_{1a_2} & X_{1a_3} & X_{1a_4} & X_{1\alpha_{ef}} \\ X_{2a_0} & X_{2a_1} & X_{2a_2} & X_{2a_3} & X_{2a_4} & X_{2\alpha_{ef}} \\ X_{3a_0} & X_{3a_1} & X_{3a_2} & X_{3a_3} & X_{3a_4} & X_{3\alpha_{ef}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X_{na_0} & X_{na_1} & X_{na_2} & X_{na_3} & X_{na_4} & X_{n\alpha_{ef}} \end{bmatrix} \quad (9)$$

The sensitivity coefficients studied here are calculated by the following expression:

$$X_{j\delta} = \frac{\partial T\left(t_j; a_0, a_1, a_2, a_3, a_4, \alpha_{ef}\right)}{\partial \delta} \text{ para j} = 1, 2, \ldots, n; \text{ and } \delta = a_0, a_1, a_2, a_3, a_4, \alpha_{ef} \quad (10)$$

To solve the non-linear system of algebraic equations, Levenberg-Marquardt iterative algorithm is used, which is based upon expanding $\mathbf{T}(\boldsymbol{\beta})$ in a Taylor series to the first-order terms and adding the Levenberg-Marquardt parameter λ. Beck and Arnold (1977) present the following formula to compute the search direction for the parameters β :

$$\boldsymbol{\beta}^{(q+1)} = \boldsymbol{\beta}^{(q)} + \left[\mathbf{X}^{T(q)}\boldsymbol{\psi}^{-1}\mathbf{X}^{(q)} + \lambda^{(q)}\mathbf{I}\right]^{-1}\left[\mathbf{X}^{T(q)}\boldsymbol{\psi}^{-1}\left(\mathbf{T_E} - \mathbf{T}(\boldsymbol{\beta})^{(q)}\right)\right] \tag{11}$$

where the superscript q is the iteration index.

As stated by Tang and Araki (2000), the solution of the inverse problem starts with a suitable guess for $\boldsymbol{\beta}^{(0)}$ vector and the iterations are continued until the condition below is satisfied:

$$\left|\beta_m^{(q+1)} - \beta_m^{(q)}\right| < \xi;\ m = 1, 2, \ldots, p \text{, where } \xi \text{ is a small, positive number.} \tag{12}$$

Previously to the inverse problem solution, computational codes have been elaborated for numerical simulation as well as for reduced sensitivity coefficients calculus. After the sensitivity analysis of the studied parameters, a specific code was developed for their estimation. In order to provide support to the main programs and sub-routines developed, the following sub-routines, described by Press *et al.* (1989), were employed: MRQMIN, MRQCOF, FGAUSS, COVSRT, GAUSSJ, GASDEV and RAN1.

5. Results

5.1. Direct problem solution

Direct problem solution conducted to the obtainment of transient temperature profiles for sensors 1 and 2 using selected input information. This information reunites all geometrics dimensions already mentioned, the heat power $W = 1,5\,\mathrm{W}$, the adsorbent density $\rho = 612,75\,\mathrm{kg/m^3}$ and the average environmental temperature $T_{initial} = 25^{\circ}\mathrm{C}$. The chosen value for W is in agreement with those ones used in the experiments conducted by Pereira *et al.* (1991), Gurgel and Klüppel (1996) as well as Gurgel *et al.* (2001), which are 0,72W - 3,72W and 1,393W - 6,811W, respectively.

According to Biloe *et al.* (2001), the effective thermal conductivity for activated carbon/pure methane packed beds is $k_b = 0,2\,\mathrm{W/(m \cdot K)}$. Sonntag *et al.* (2001) as well as Kreith and Bohn (2003) recommend $c_p = 1260\,\mathrm{J/(kg \cdot K)}$ for carbon. Kreith and Bohn (2003) present that for this specific heat value, thermal conductivity value, $k_b = 0,238\,\mathrm{W/(m \cdot K)}$, is quite approximate to that one suggested by Biloe *et al.* (2001). The mentioned values for k_b, ρ and c_p made possible to calculate the effective thermal diffusivity real value, which is $\alpha_{ef} = 2,59 \cdot 10^{-7}\,\mathrm{m^2/s}$.

The quartic polynomial coefficients that represent transient temperature profile at r_2 are: $a_0 = 24,80112444^{\circ}\mathrm{C}$; $a_1 = 0,002325632\,^{\circ}\mathrm{C/s}$; $a_2 = -4,201524185 \cdot 10^{-7}\,^{\circ}\mathrm{C/s^2}$; $a_3 = 3,638830128 \cdot 10^{-11}\,^{\circ}\mathrm{C/s^3}$ and $a_4 = -1,212259522 \cdot 10^{-15}\,^{\circ}\mathrm{C/s^4}$. These values are obtained from a fit of the solution, at r_2 position, for this problem under different boundary conditions such as: heat flow at the centre of the cylindrical cavity and forced convection at the cylindrical external wall. Thermograms exposed on Fig. 2 are plotted for a 3 hour (10800s) heating period, using $\Delta t = 1$ s as time increment.

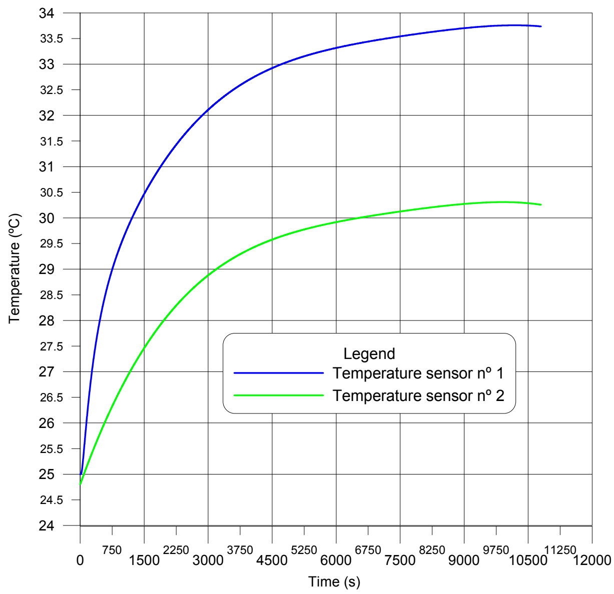

Figure 2. Behaviour of the thermograms for sensors 1 and 2 at a 3 hour heating period

5.2. Numerical simulation and sensitivity analysis

A computational simulation is performed in order to obtain the experimental transient temperature profile for sensor nº 1 at noise values of 1% and 3%, respectively, as shown in Fig. 3:

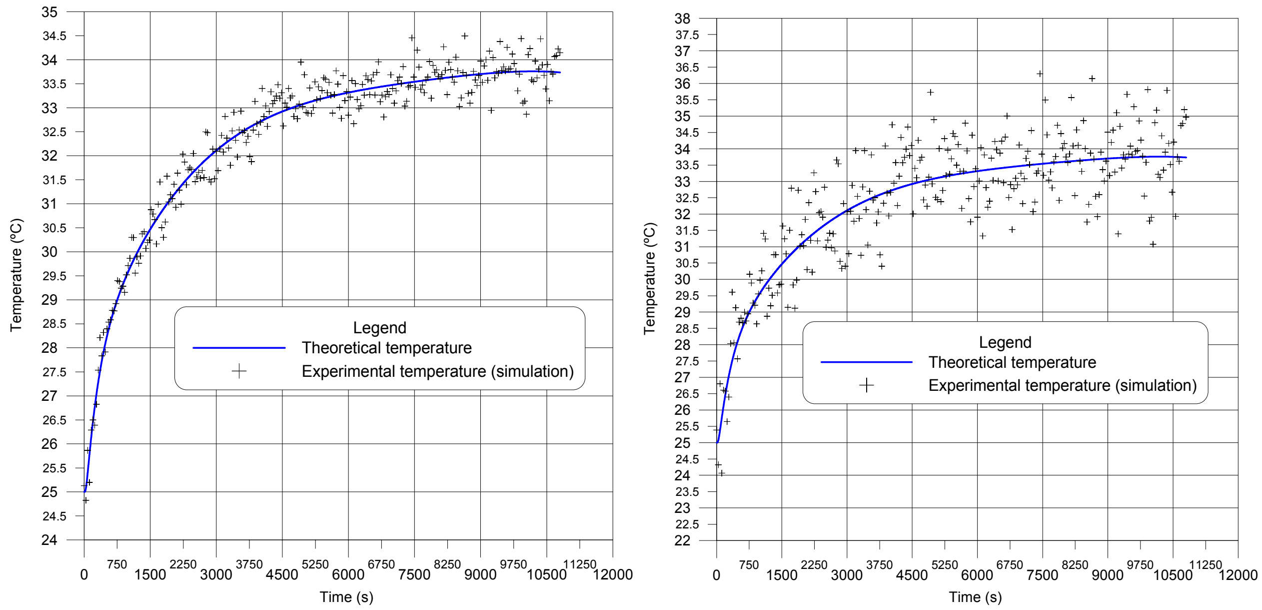

Figure 3. Sensor nº 1 experimental thermogram simulation for different noise values: (3.a) 0,01ºC (left) and (3.b) 0,03ºC (right) at a 3 hour heating period

Additionally, a parameter sensitivity analysis is also performed for sensor nº 1 (located at the 15º nodal point of the structured mesh) by plotting the reduced sensitivity coefficients (RSC), dependents on time (Fig. 4.a):

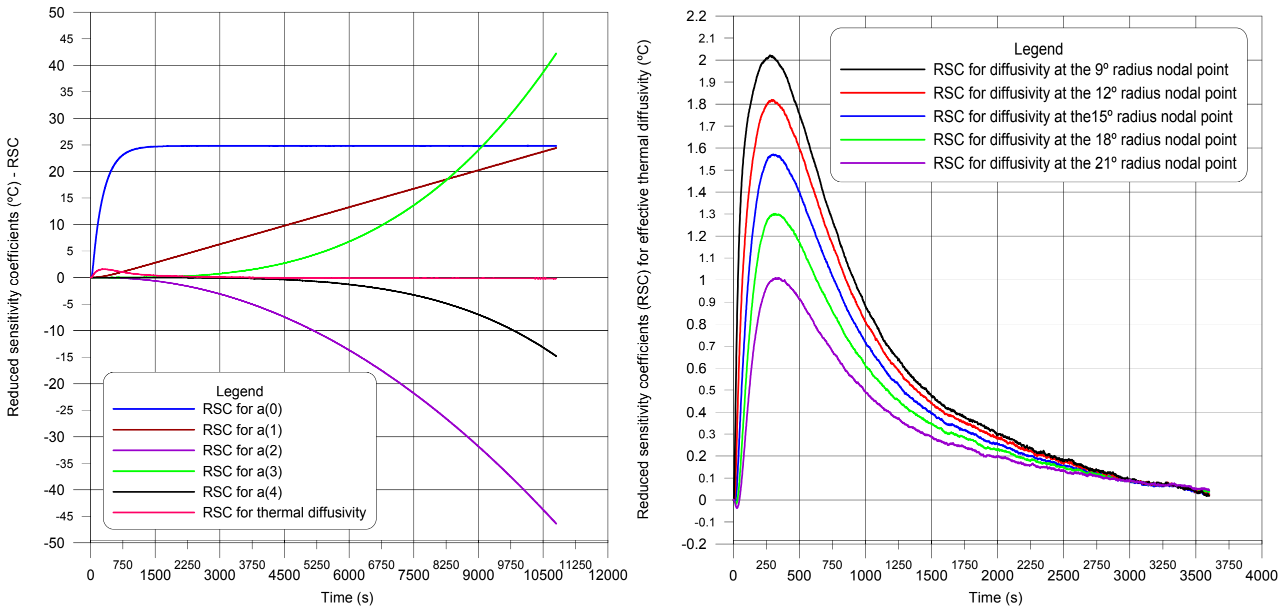

Figure 4. (4.a) Reduced sensitivity coefficients behaviour for the parameters studied during a 3 hour heating period (left) and (4.b) effective thermal diffusivity sensitivity, related to radial position, during an 1 hour heating period (right)

The sensitivity analysis guided to notice that reduced sensitivity coefficients for parameters a_0, a_1, a_2, a_3, a_4 and α_{ef} presented a well defined linear independence. RSC values for parameters a_1, a_2, a_3 and a_4, increased considerably as time evolves. For parameter a_0, RSC values are high and maintained itself constant after the first 1500s

(25 minutes). Referring to parameter α_{ef} , sensitivity is expressed only in the first 1500s, reaching values near to zero in the rest of the time period studied.

Effective thermal diffusivity sensitivity, related to radial position, is also analysed (Fig. 4.b). This analysis revealed that $\frac{\partial T}{\partial \alpha_{ef}}$ values are continuously crescent for mesh nodal points adjacent to the electrical resistance (first nodal point of the structured mesh). Therefore, it is justified the choice to solve the inverse problem, estimating the effective thermal diffusivity as well as the quartic polynomial coefficients, for sensor nº 1 which is the most close to the resistance, in real terms. Based on the aspects discussed, one can affirm that reliable conditions for parameter estimation are satisfied.

5.3. Inverse problem solution

To achieve the inverse problem solution, all input information as well as the assumptions reported before are considered. Those were previously used in the numerical simulation and sensitivity analysis. The choice of suitable initial guesses, which have approximate magnitudes in comparison to the exact value of parameters, is particularly relevant due its contribution to improve convergence velocity and reduce computational cost, in terms of number of iterations and memory capacity. Thereby, using suitable initial values it is possible determine the effective thermal diffusivity and quartic polynomial coefficients values. Table 1 presents the initial values chosen, the exact values (already presented in 5.1), the estimated values and the uncertainties related to them. The estimation is developed with three different error values introduced. In addition to this, values for the minimized statistic χ^2 and the Levenberg-Marquardt parameter λ are determined once they represent indicators of the estimation convergence.

Table 1. Estimated values and uncertainties related to the parameters studied.

Estimation with 1% error - 10 iterations; Chi-square statistic = 10753,40; Lambda = 1E-08						
Parameters	**a_0 [ºC]**	**a_1 [ºC/s]**	**a_2 [ºC/s²]**	**a_3 [ºC/s³]**	**a_4 [ºC/s⁴]**	**α(ef) [m²/s]**
Initial values	31,8011	1,9060E-04	-3,1213E-09	4,2788E-09	-1,0025E-17	8,5000E-08
Estimated values	24,8235	2,3075E-03	-4,1692E-07	3,6258E-11	-1,2167E-15	2,5681E-07
Exact values	24,8011	2,3256E-03	-4,2015E-07	3,6388E-11	-1,2123E-15	2,5900E-07
Uncertainties (±)	4,9710E-02	4,0838E-05	1,2844E-08	1,6438E-12	7,2550E-17	5,4122E-09
Estimation with 3% error - 10 iterations; Chi-square statistic = 10808,21; Lambda = 1E-08						
Parameters	**a_0 [ºC]**	**a_1 [ºC/s]**	**a_2 [ºC/s²]**	**a_3 [ºC/s³]**	**a_4 [ºC/s⁴]**	**α(ef) [m²/s]**
Initial values	31,8011	1,9060E-04	-3,1213E-09	4,2788E-09	-1,0025E-17	8,5000E-08
Estimated values	24,8453	2,2652E-03	-4,0984E-07	3,5996E-11	-1,2272E-15	2,4971E-07
Exact values	24,8011	2,3256E-03	-4,2015E-07	3,6388E-11	-1,2123E-15	2,5900E-07
Uncertainties (±)	0,154127	1,4143E-04	4,5134E-08	5,8096E-12	2,5624E-16	1,6850E-08
Estimation with 5% error - 12 iterations; Chi-square statistic = 10910,00; Lambda = 1E-08						
Parameters	**a_0 [ºC]**	**a_1 [ºC/s]**	**a_2 [ºC/s²]**	**a_3 [ºC/s³]**	**a_4 [ºC/s⁴]**	**α(ef) [m²/s]**
Initial values	31,8011	1,9060E-04	-3,1213E-09	4,2788E-09	-1,0025E-17	8,5000E-08
Estimated values	24,8529	2,1945E-03	-3,9461E-07	3,4722E-11	-1,1941E-15	2,3807E-07
Exact values	24,8011	2,3256E-03	-4,2015E-07	3,6388E-11	-1,2123E-15	2,5900E-07
Uncertainties (±)	0,250679	2,0899E-04	6,4944E-08	8,2563E-12	3,6255E-16	2,5331E-08

The comparison between the values presented in Tab. 1 indicates that the estimation is very good for noise value of 1%. Specifically for this test the estimated values are quite similar to the exact ones and small magnitude uncertainties for each one of the parameters have being achieved. For noise value of 3% it is verified the occurrence of acceptable deviates related to the exact value of the parameters as well as progressing uncertainties, particularly for parameter a_0. Further tests with the same initial values were realized demonstrating that whenever higher noise values $(\geq 5\%)$ are used the estimation becomes unsatisfactory. The chosen trial values are relatively distant from the exact ones, confirming the estimation accuracy. Tests using different initial guesses were performed as well revealing convergence to the exact solution when suitable magnitude values are selected for these guesses. These tests also indicated that for very distant initial values the convergence is significantly damaged. In fact, according to Press *et al.* (1989), this is expected when one is dealing with a non-linear optimization problem considering unsuitable trial values.

6. Conclusions

Based on the arguments presented, one can conclude that the direct problem solution contributed for the comprehension of the time dependent temperature profile behaviour of the porous packed bed, in each one of the sensors considered. Sensitivity analysis made possible to understand the influence of each parameter in the simultaneous estimation as well as their behaviour during the progress of time, assisting the decision making process concerning what transient section of the thermogram should be used in the activated carbon/pure methane gas pair parameter estimation. Inverse problem solution made possible this estimation. Mathematical modelling coupled with the computational codes developed formed the structure that provided support to the achievements above mentioned. The results obtained are significant and constitute a helpful tool for the development of forthcoming experiments, contributing to assure the reliability and accuracy of future results to be achieved. The original contribution of the present work beyond other works in the literature - particularly those performed by Gurgel and Grenier (1990), Pereira *et al.* (1991), Gurgel and Klüppel (1996) and Gurgel *et al.* (2001) - is the simultaneous estimation of the second boundary condition of the problem and the effective thermal diffusivity in a simulated adsorptive porous media considering the experimental setup used by the mentioned authors.

7. Acknowledgements

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9. Responsibility notice

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