#### PARAMETER INVERSE PROBLEM OF **ESTIMATION** IN AN SIMULTANEOUS HEAT AND MASS TRANSFER IN **ONE-**A **DIMENSIONAL POROUS MEDIUM**

# Jader Lugon Jr.

SENAI/RJ, Agência de Formação Profissional de Itaperuna Av. Dep. José de Cerqueira Garcia, 883 CEP 28300-000, Itaperuna, Rio de Janeiro, Brazil. jljunior@firjan.org.br

Computational Modelling Program Instituto Politécnico Universidade do Estado do Rio de Janeiro CP 97282, 28.601-970, Nova Friburgo, RJ, Brazil lugon@iprj.uerj.br

## Antônio J. Silva Neto

Department of Mechanical Engineering and Energy Instituto Politécnico Universidade do Estado do Rio de Janeiro CP 97282, 28601-970, Nova Friburgo, RJ, Brazil ajsneto@iprj.uerj.br

**Abstract.** In the present work we deal with the analysis, formulation and solution of an inverse heat and mass transfer problem in a one-dimensional porous medium. The direct problem is formulated with Luikov's equations which are solved using the finite difference method. The inverse problem is formulated implicitly and is solved using the Levenberg-Marquardt method. A preliminary sensitivity analysis is performed and the relevant model parameters are then estimated.

Key-words: Inverse problems, Heat and mass transfer, drying, Luikov equations.

## 1. Introduction

The analysis of the simultaneous heat and mass transfer phenomena in porous media has several relevant applications in different areas such as mechanical, biomedical and environmental engineering. Just to mention a few examples (Mikhailov and Özisik, 1984): (i) modeling of the wicks of heat pipes; (ii) analysis of drying process of structural concrete parts; (iii) drying of human blood plasma; and (iv) pollutant migration in soil.

Just to mention a few works on the subject, Dolinskiy et al. (1991) developed a model for the conjugate problem of heat and mass transfer between a heat transfer agent and a material that is continuously pulled through it, and Dietl et al. (1998) developed models for both the direct and inverse problems to predict the drying behavior of capillary porous, hygroscopic materials, and compared the results with experimental data.

Luikov (1966, 1975) observed experimentally that the moisture migration in a drying process is governed by the temperature gradient. Then using concepts from irreversible processes thermodynamics he was able to derive the now called Luikov equations, used for the mathematical modeling of the phenomena of simultaneous heat and mass transfer in porous media. Some analytical solutions are available in the literature (Mikhailov, 1975, Brown, 1989). Hybrid Methods have also been used. Mikhailov and Özisik (1984) used the integral transform method, and Cotta (1993) developed and used the generalized transform integral technique. Thum et al. (1998) used the GITT and the Laplace transform for the solution of the resulting ordinary differential equations for the Luikov's problem in two-dimensional media.

In the direct problem the solution of two coupled partial differential equations with the proper boundary and initial conditions leads to the determination of both temperature and moisture distributions within the porous medium. Orlande (2002) and Dantas et al. (2002, 2003) have addressed the inverse problem of parameter estimation in heat and mass transfer in a porous medium. The direct problem is modeled with the Luikov's equations which are solved using the GITT, generalized integral transform method (Cotta, 1993). An implicit formulation is used for the inverse problem, and it is solved using the Levenberg-Marquardt method.

Silva Neto and co-workers (Lugon et al., 2002, 2002a) have addressed independently the same problem using also Luikov's equations for the mathematical formulation of the direct problem and the solution of the inverse problem, but in their work the solution of the direct problem is obtained with the finite difference method, instead of the generalized integral transform technique. Another difference is also the time frame used for the analysis of the direct and inverse problems. Dantas et al. (2002, 2003) considered a dimensionless time up to  $\tau = 120$ , while Silva Neto and co-workers considered times up to  $\tau = 1$ , which for samples of porous media we are interested in, with 50 mm

thickness, represents 1 hour of real time experiment. For such samples the preliminary sensitivity analysis performed indicates that most of the relevant phenomena is observed within that time frame.

Huang and Yeh (2002) investigated the same problem. They have also used a finite difference approximation for the solution of the direct problem, and the inverse problem was solved using Alifanov's iterative regularization method (Alifanov et al, 1995). These authors have also considered the final time of observation  $\tau = 1$ .

In the present work we go a step further on the work done by Lugon et al. (2002, 2002a). The direct problem is mathematically formulated with Luikov's equations which are solved using the finite difference method. The inverse problem is formulated implicitly (Silva Neto, 2002), as an optimization problem, and is solved using the deterministic gradient based (Silva Neto and Soeiro, 2001, 2003) Levenberg-Marquardt method (Silva Neto and Moura Neto, 1999). Here we look into the estimation of the phase change criterion, and Luikov, Possnov and Kossovitch dimensionless numbers. Besides the mathematical formulation of both the direct and inverse problems, test case results are presented.

# 2. Mathematical formulation and the solution of the Direct Problem

In accordance with the schematic representation shown in Fig. 1, consider the problem of simultaneously heat and mass transfer in a one-dimensional porous media in which heat is supplied to the left surface of the porous media, at the same time that dry air flows over the right surface.

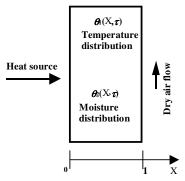


Figure 1 – Drying process schematic representation

The mathematical formulation of the direct heat and mass transfer problem considered, in the dimensionless form, is given by (Mikhailov and Özisik, 1984, Cotta, 1993)

$$\frac{\partial \theta_1(X,\tau)}{\partial \tau} = \alpha \frac{\partial^2 \theta_1}{\partial X^2} - \beta \frac{\partial^2 \theta_2}{\partial X^2}, \quad 0 < X < 1, \quad \tau > 0$$
(1a)

$$\frac{\partial \theta_2(X,\tau)}{\partial \tau} = Lu \frac{\partial^2 \theta_2}{\partial X^2} - Lu Pn \frac{\partial^2 \theta_1}{\partial X^2}, \quad 0 < X < 1, \quad \tau > 0$$
(1b)

subject to the initial conditions

 $\theta_1(X,0) = 0, \qquad 0 \le X \le 1 \tag{2a}$ 

 $\theta_2(X,0) = 0, \qquad 0 \le X \le 1 \tag{2b}$ 

and to the boundary conditions

$$\frac{\partial \theta_1(0,\tau)}{\partial X} = -Q, \quad \tau > 0 \tag{3a}$$

$$\frac{\partial \theta_2(0,\tau)}{\partial X} = -PnQ, \quad \tau > 0 \tag{3b}$$

$$\frac{\partial \theta_1(1,\tau)}{\partial X} + Bi_q \theta_1(1,\tau) = Bi_q - (1-\varepsilon) Ko Lu Bi_m [1-\theta_2(1,\tau)] = 0, \quad \tau > 0$$

$$\frac{\partial \theta_2(1,\tau)}{\partial X} + Bi_m^* \theta_2(1,\tau) = Bi_m^* - Pn Bi_q [\theta_1(1,\tau)-1], \quad \tau > 0$$
(3d)

where  $\alpha = 1 + \varepsilon$  Ko Lu Pn,  $\beta = \varepsilon$  Ko Lu,  $Bi_m^* = Bi_m [1 - (1 - \varepsilon)Pn \text{ Ko } Lu]$ , and the dimensionless variables are defined as

$$\theta_{1}(X,\tau) = \frac{T(x,t) - T_{0}}{T_{s} - T_{0}}, \text{ temperature} \qquad Pn = \delta \frac{T_{s} - T_{0}}{u_{0} - u^{*}}, \text{ Possnov number}$$

$$\theta_{2}(X,\tau) = \frac{u_{0} - u(x,t)}{u_{0} - u^{*}}, \text{ moisture} \qquad Ko = \frac{r}{c} \frac{u_{0} - u^{*}}{T_{s} - T_{0}}, \text{ Kossovitch number}$$

$$X = \frac{x}{l}, \text{ spatial coordinate} \qquad Bi_{q} = \frac{hl}{k}, \text{ heat Biot}$$

$$\tau = \frac{at}{l^{2}}, \text{ time} \qquad Bi_{m} = \frac{h_{m}l}{k_{m}}, \text{ mass Biot}$$

$$Lu = \frac{a_{m}}{a}, \text{ Luikov number} \qquad Q = \frac{ql}{k(T_{s} - T_{0})}, \text{ heat flux}$$

and *a* represents the thermal diffusivity of the porous medium,  $a_m$  the moisture diffusivity of the porous media, *c* the specific heat of the porous medium, *h* the heat transfer coefficient between the porous medium and the air,  $h_m$  the mass transfer coefficient between the porous medium and the air, *k* the thermal conductivity,  $k_m$  the moisture conductivity, *l* the width of the medium, *q* the thermal flux supplied at the porous medium left side, *r* the latent heat of evaporation,  $T_0$  the initial uniform temperature of the porous medium,  $T_s$  the dry air initial temperature,  $u_0$  the initial moisture content,  $u^*$  the equilibrium temperature with the air, *x* the coordinate axis,  $\varepsilon$  the phase change criterion (*i.e.*,  $\varepsilon = 1$ , vapor,  $\varepsilon = 0$ , liquid) and  $\delta$  is the thermogradient coefficient.

When the geometry, the initial and boundary conditions, and the medium properties are known, the system of equations (1-3) can be solved yielding the temperature and moisture distribution in the media. In this work the finite difference method is used to solve the system (1-3).

## 2.1 Direct Problem Solution

The solution of a partial differential equation (PDE) in a given domain implies in the determination of the values for the dependent variable in each point of the region. For the implementation of a finite difference approximation the physical domain is discretized, being then represented through a computational grid (see Fig. 2).

The derivatives in the differential equations and in the boundary conditions are then approximated through finite differences resulting in a system of linear algebraic equations for the temperature  $\theta_1$ , and for the moisture  $\theta_2$ , at the nodal points.

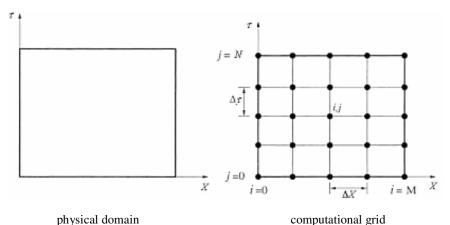


Figure 2 – Physical domain and computational grid

Using a forward difference approximation for the first derivative in time in Eq. (1a) and a centered difference approximation for the second derivative in space for both  $\theta_1$  and  $\theta_2$ , one obtains from Eq. (1a)

$$-\alpha\Delta\tau\theta_{1}(X_{i-1},\tau_{j+1}) + (\Delta X^{2} + 2\alpha\Delta\tau)\theta_{1}(X_{i},\tau_{j+1}) - \alpha\Delta\tau\theta_{1}(X_{i+1},\tau_{j+1}) =$$

$$= \Delta X^{2}\theta_{1}(X_{i},\tau_{j}) - \beta\Delta\tau\theta_{2}(X_{i-1},\tau_{j+1}) + 2\beta\theta_{2}(X_{i},\tau_{j+1}) - \beta\Delta\tau\theta_{2}(X_{i+1},\tau_{j+1})$$

$$\tag{4}$$

At node i = 0 (see Fig. 2), Eqs. (3<sup>a</sup>-b) are approximated in Eq. (4) resulting in

$$\left(\Delta X^{2} + 2\alpha\Delta\tau\right)\theta_{1}(X_{0},\tau_{j+1}) - 2\alpha\Delta\tau\theta_{1}(X_{1},\tau_{j+1}) = 2\alpha\Delta\tau\Delta XQ + \Delta X^{2}\theta_{1}(X_{0},\tau_{j}) - 2\beta\Delta\tau\Delta\tau\Delta XPn Q + 2\beta\Delta\tau\theta_{2}(X_{0},j_{j+1}) - 2\beta\Delta\tau\theta_{2}(X_{1},\tau_{j+1})\right)$$
(5)

Using the same procedure for node i = M, Eqs (3c-d) are approximated and also substituted in Eq. (4)

$$-2\alpha\Delta\tau\theta_{1}(X_{M-1},\tau_{j+1}) + (\Delta X^{2} + 2\alpha\Delta\tau + 2\alpha\Delta\tau\Delta X Bi_{q})\theta_{1}(X_{M},\tau_{j+1}) =$$

$$= \alpha\Delta\tau\{2\Delta X Bi_{q} - 2\Delta X(1-\varepsilon)Ko Lu Bi_{m}[1-\theta_{2}(X_{M},\tau_{j})]] + \Delta X^{2}\theta_{1}(X_{M},\tau_{j}) - \beta\Delta\tau\{\theta_{2}(X_{M-1},\tau_{j+1}) - 2\theta_{2}(X_{M},\tau_{j+1}) + \theta_{2}(X_{M-1},\tau_{j}) - 2\Delta X Bi_{m}^{*}\theta_{2}(X_{M},\tau_{j}) + 2\Delta X Bi_{m}^{*} - Pn Bi_{q}[\theta_{1}(X_{M},\tau_{j}) - 1]\}$$
(6)

Using forward difference in time and centered difference in space Eq. (1b) is approximated by

$$-\Delta\tau \operatorname{Lu}\theta_{2}(X_{i-1},\tau_{j+1}) + (\Delta X^{2} + 2\operatorname{Lu}\Delta\tau)\theta_{2}(x_{i},\tau_{j+1}) - \operatorname{Lu}\Delta\tau\theta_{1}(X_{i+1},\tau_{j+1}) = = \Delta X^{2}\theta_{2}(X_{i},\tau_{j+1}) - \Delta\tau \operatorname{LuPn}[\theta_{1}(X_{i-1},\tau_{j+1}) - 2\theta_{1}(X_{i},\tau_{j+1}) + \theta_{1}(X_{i+1},\tau_{j+1})]$$
(7)

At node i = 0, using again the developed approximations for Eqs. (3a-b) and substituting in Eq. (7) results

$$\left(\Delta X^{2} + 2Lu\Delta\tau\right)\theta_{2}\left(X_{0}, \tau_{j+1}\right) - 2\Delta\tau Lu\theta_{2}\left(X_{1}, \tau_{j+1}\right) = 2\Delta\tau Lu Pn Q\Delta X + \Delta X\theta_{2}\left(X_{0}, \tau_{j}\right) - \Delta\tau Lu Pn \left[2\theta_{1}\left(X_{1}, \tau_{j+1}\right) + 2Q\Delta X - 2\theta_{1}\left(X_{0}, \tau_{j+1}\right)\right]$$

$$(8)$$

At node i = M, substituting in Eq. (7) the developed approximations for Eqs. (3a-b) leads to

$$- 2\Delta\tau Lu \ \theta_2 (X_{M-1}, \tau_{j+1}) + (\Delta X^2 + 2Lu \ \Delta\tau + 2\Delta\tau\Delta X \ Lu \ Bi_m^*) \theta_2 (X_M, \tau_{j+1}) = = \Delta\tau Lu \{2\Delta X \ Bi_m^* - 2\Delta X \ Pn \ Bi_q [\theta_1 (X_M, \tau_j) - 1]\} + \Delta X^2 \theta_2 (X_M, \tau_j) - - \Delta\tau Lu \ Pn \{\theta_1 (X_{M-1}, \tau_{j+1}) - \theta_1 (X_M, \tau_{j+1}) + \theta_1 (X_{M-1}, \tau_j) + + 2\Delta X \ Bi_q \theta_1 (X_M, \tau_j) + 2\Delta X \ Bi_q - 2\Delta X (1 - \varepsilon) Ko \ Lu \ Bi_m [1 - \theta_2 (X_M, \tau_j)]\}$$
(9)

Equations (4-9) form a complete set that allows the determination of the temperature and moisture content at the grid nodes represented in Fig. 3. We are using an implicit finite difference formulation.

#### 2.2 Validation of the Direct Problem solution

In order to validate the results obtained with the solution of the direct problem implemented with the FDM, they were compared with the results presented by Cotta (1993). The parameters used were: Lu = 0.4, Pn = 0.6,  $\varepsilon = 0.2$ , Ko = 5.0,  $Bi_m = Bi_q = 2.5$  and Q = 0.9.

In Figs. 3 and 4 it can be observed that the results for the direct problem are in good agreement with those obtained by Cotta (1993), Lobo et al. (1987) and Mikhailov and Özisik (1984).

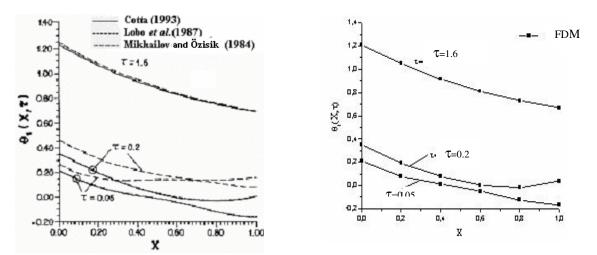


Figure 3 – Dimensionless temperature distribution Lu = 0.4, Pn = 0.6,  $\varepsilon = 0.2$ , Ko = 5.0,  $Bi_m = Bi_q = 2.5$  and Q = 0.9. (The results shown in the figure on the left were extracted from the book by Cotta, 1993).

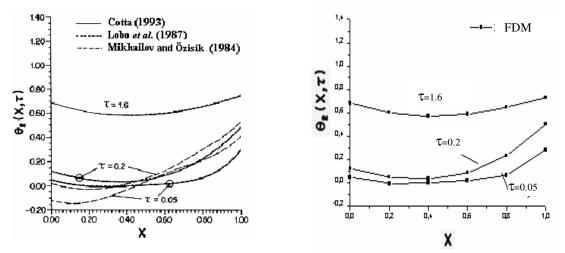


Figure 4 – Dimensionless moisture distribution Lu = 0.4, Pn = 0.6,  $\varepsilon = 0.2$ , Ko = 5.0,  $Bi_m = Bi_q = 2.5$  and Q = 0.9. (The results shown in the figure on the left were extracted from the book by Cotta, 1993).

#### **3.** Preliminary sensitivity analysis

The sensitivity analysis plays a major role in several aspects related to the formulation and solution of an inverse problem, i.e. from the first steps on the preparation of an experimental apparatus (Beck and Arnold, 1977, Taktak et al., 1993, Emery et al., 1993), in the study of the effects of the model parameters on the state variable that can be measured (Dowding et al., 1999), and finally in the solution of the inverse problem itself (Tseng et al., 1995).

In all cases it is required the computation of the sensitivity coefficients. These coefficients are defined as

$$SC_{P_j}(X,\tau) = \frac{\partial V(X,\tau)}{\partial P_j}, \quad j = 1, 2, \cdots, N$$
 (10)

where V is the state variable,  $P_i$ , is a particular unknown of the problem and N is the total number of unknowns.

In the present work the state variable is the temperature  $\theta_1$ , and the unknowns are: P<sub>1</sub>=Lu, P<sub>2</sub>=Pn, P<sub>3</sub>= $\epsilon$ , P<sub>4</sub>=Ko, P<sub>5</sub>=Bi<sub>m</sub> and P<sub>6</sub>=Bi<sub>q</sub>.

There are several ways to calculate the sensitivity coefficients. Blackwell et al. (1999) derived the sensitivity equations for heat conduction problems by differentiating the energy equation with respect to the parameter of interest, and then solved the resulting sensitivity equations numerically. Meric (1998) investigated a shape optimization

problem, and used the adjoint variable method for the sensitivity analysis. Here we use a finite difference approximation for Eq. (10).

As a general guideline the sensitivity of the state variable to the parameter we want to estimate must be high enough to allow an estimative within reasonable confidence bounds. Moreover, when two or more parameters are simultaneously estimated, their effects on the state variable must be independent (uncorrelated). Therefore, when represented graphically the sensitivity coefficients should not have the same shape. If they do it means that two or more different parameters affect the state variable in the same way, being difficult to distinguish their influences separately which yields to poor estimations.

So far we have done only a preliminary computation and analysis of the sensitivity coefficients for the model parameters  $P_{j}$ , j = 1, 2, ..., 6, on the state variable  $\theta_l(X, \tau)$ , with  $0 \le X \le 1$  and  $0 \le \tau \le \tau_f$ , where  $\tau_f = 1$ . The results of such preliminary analysis on the sensitivity coefficients  $SC_{P_j}(X, \tau)$ , for j=1,2,...,6, are represented in Figs. 5-10 as

a function of the dimensionless spatial coordinate X and dimensionless time  $\, au$  .

In Figs. 5-7 we observe a high sensitivity to Lu, Po and  $\varepsilon$ , mainly if the temperature sensor is located at X = 1. The sensitivity to Ko is represented in Fig. 8, and is smaller than those presented before, but still may allow a good estimation for such parameter. The sensitivities to Bi<sub>m</sub> and Bi<sub>q</sub> are represented in Figs. 9 and 10, respectively. These sensitivities are much smaller than those for the other parameters, what makes the estimation difficult, and besides that they present the same shape, probably yielding to unreliable estimates if one attempts to perform a simultaneous estimation of such parameters.

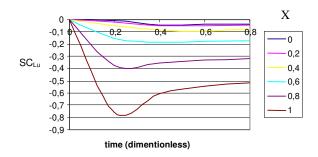


Figure 5 - Sensitivity coefficients for Luikov number

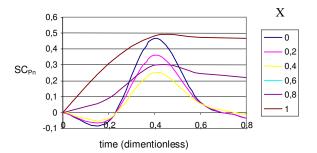


Figure 6 - Sensitivity coefficients for Possnov number

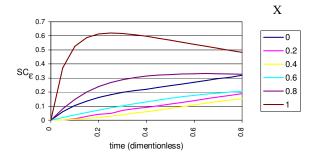


Figure 7 - Sensitivity coefficients for phase change criterion

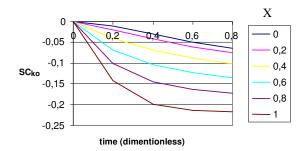


Figure 8 - Sensitivity coefficients for Kossovitch number

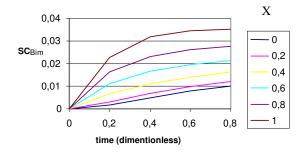


Figure 9 - Sensitivity coefficients for mass Biot

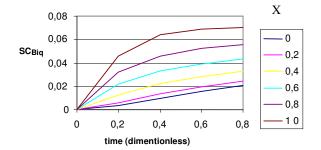


Figure 10 - Sensitivity coefficients for heat Biot

# 4. Mathematical formulation and solution of the Inverse Problem

# 4.1 Inverse Problem Formulation

In accordance with the sensitivity analysis presented in the previous section we will focus on the estimation of Lu, Pn, Ko and  $\varepsilon$ . For that purpose it is considered that transient temperature measurements taken in different locations of the medium are available.

Since the number of experimental data, M, is larger than the number of unknowns to be estimated, N=4, the inverse problem is implicitly formulated (Silva Neto, 2002) as a finite dimensional optimization problem where we seek for the minimization of the functional of squared residues

$$S = \sum_{i=1}^{M} \left[ \theta_{1i}(\vec{P}) - Y_i \right]^2 = \vec{F}^T \vec{F}$$
(11)

where  $Y_i$  represents the dimensionless temperature measured in the porous media,  $\theta_{1i}(\vec{P})$  the calculated temperature, M is the number of experimental data available,  $\vec{P}$  is the vector of unknowns and  $F_i = \theta_{1i}(\vec{P}) - Y_i$ , i = 1, 2, ..., M.

#### 4.2 Inverse problem solution

For the solution of the simultaneous heat and mass transfer inverse problem under analysis it was used the Levenberg-Marquardt method (Silva Neto and Moura Neto, 1999).

In order to minimize the functional S we first write

$$\frac{dS}{d\vec{P}} = \frac{d}{d\vec{P}} \left(\vec{F}'\vec{F}\right) = 0 \quad \rightarrow \quad J'\vec{F} = 0 \tag{12}$$

where J is the Jacobian matrix, with the elements  $J_{ps} = \partial \theta_{1p} / \partial P_s$  being p = 1, 2, ..., M, and s = 1, 2, ..., N. Observe that the elements of the Jacobian matrix correspond to the sensitivity coefficient presented in the previous section.

Using a Taylor's expansion and keeping only the terms up to the first order,

$$\vec{F}(\vec{P} + \Delta \vec{P}) \cong F(\vec{P}) + J\Delta \vec{P}$$
<sup>(13)</sup>

Introducing the above expansion in Eq. (11) results

$$J^{T} J \Delta \vec{P} = -J^{T} \vec{F} \left( \vec{P} \right)$$
<sup>(14)</sup>

In the Levenberg-Marquardt method it is added to the diagonal of matrix  $J^T J$  a damping  $\lambda^n$  factor to help to achieve convergence (Marquardt, 1963).

Equation (13) is written in a more convenient form to be used in the iterative procedure,

$$\Delta \vec{P}^{n} = -\left[ \left( J^{n} \right)^{T} J^{n} + \lambda^{n} \vec{I} \right]^{-1} \left( J^{n} \right)^{T} \vec{F} \left( \vec{P}^{n} \right)$$
(15)

where  $\breve{I}$  is the identity matrix and n is the iteration counter

The iterative procedure starts with an estimate for the unknown parameters,  $\vec{P}^0$ , being new estimates obtained with  $\vec{P}^{n+1} = \vec{P}^n + \Delta \vec{P}^n$ , while the corrections  $\Delta \vec{P}^n$  are calculated with Eq. (15). This iterative procedure is continued until a convergence criteria such as

$$\left|\Delta P_k^n / P_k^n\right| < \varepsilon, \qquad n = 1, 2, \cdots, N \tag{16}$$

is satisfied, where  $\varepsilon$  is a small number, e.g.  $10^{-5}$ .

The elements of the Jacobian matrix, as well as the right side term of Eq. (14), are calculated at each iteration using the solution of the problem with the estimates for the unknowns obtained in the previous iteration.

# 4.2 Confidence bounds

The confidence bounds for the estimates  $\vec{P}$  are calculated using the procedure developed by Gallant (1987). Using the notation employed by Huang and Özisik (1990).

$$\sigma_{\vec{p}} = \sigma \left\{ diag \left[ \frac{\partial \vec{\theta}_{1}^{T}}{\partial \vec{P}} \frac{\partial \theta_{1}}{\partial \vec{P}^{T}} \right]^{-1} \right\}^{\frac{1}{2}}$$
(17)

where  $\vec{\theta}_1$  is the vector containing the elements  $\vec{\theta}_{1_i}$ , i = 1, 2, ..., M, and  $\sigma$  is the standard deviation of the measurement errors. Assuming a normal distribution for the experimental errors, and 99% of confidence, the confidence bounds for the estimates  $P_s$ , s = 1, 2, ..., N, are calculated by (Flach and Özisik, 1989)

$$[P_s - 2,576\sigma_s, P_s + 2,576\sigma_s], \qquad j = 1, 2, ..., N$$
<sup>(18)</sup>

### 5. Numerical results and discussion

### 5.1 Synthetic data

As real data was not available we have generated synthetic data with

$$Y_{meas_i} = \theta_{1_{exact_i}} + e\sigma \tag{19}$$

where e is a random number and  $\sigma$  is the standard deviation of measurement errors.

## 5.2 Validation of the Inverse Problem solution

In order to perform the validation of the methodology we have solved the inverse problem with noiseless data, i.e.  $\sigma = 0$  in Eq. (19). All four parameters of interest were simultaneously estimated, and the following reference test case was considered: Lu=0.4, Pn=0.6, Ko=5.0,  $\varepsilon$ =0.2. The other parameters that are included in the model but were not estimated were fixed at Q=0.9, Bi<sub>q</sub>=2.5 and Bi<sub>m</sub>=2.5.

Trying to use data for which sensitivity is the highest we have considered just one temperature sensor located at X=1 acquiring data starting at  $\tau_0 = 0.6$  at every interval  $\Delta \tau = 0.01$ , up to the final time of observation  $\tau_f = 1.0$ .

All parameters were estimated simultaneously, requiring around 30 minutes of CPU time on a Pentium II 266 MHz processor.

# 5.3 Estimation with noisy data

Two different test cases were performed using synthetic data with 3% of noise. In the first one Ko was estimated separately. The other parameters were kept in their reference values. Five different runs were performed using different sets of experimental data. In Fig. 11 are presented the estimates for the five runs with the corresponding confidence bounds. Each run required up to 10 minutes of CPU time on the same processor described before.

In Fig. 12 are presented the results obtained in the second test case estimating simultaneously Lu and Pn. In the third case the change phase criterion  $\varepsilon$  was estimated separately and the results are shown in Fig. 13.

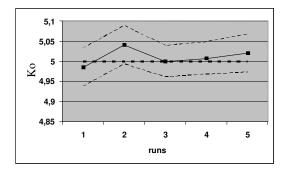


Figure 11 – Estimation of Ko in different runs.

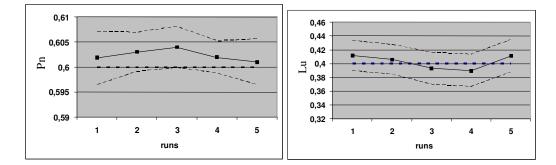


Figure 12 – Simultaneous estimation of Lu and Pn in different runs.

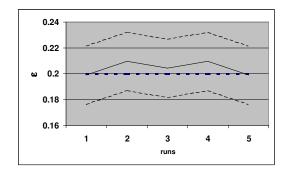


Figure 13 – Estimation of  $\varepsilon$  in different runs.

# 6. Conclusions

The Levenberg-Marquardt was successfully applied for the solution of a simultaneous heat and mass transfer inverse problem. Focus was given for the observation times up to  $\tau_f = 1$ , while other works in the literature look at longer times. This is a on going project in its preliminary stages, and a deeper investigation of the sensitivity coefficients is required because some deviation from published works was observed.

In fact our main goal is the combination of stochastic with deterministic methods for the solution of inverse heat and mass transfer problems, as used by Silva Neto and Soeiro (2001, 2003) in the solution of inverse problems of heat transfer by radiation and conduction. The implementation of the Levenberg-Marquardt algorithm was the first step in that direction, and the next step is the implementation of a genetic algorithm, which is already being performed.

# Acknowledgements

The authors acknowledge the financial support provided by CNPq, CAPES and FAPERJ.

# REFERENCES

- Alifanov, O. M., Artyukhin, E. A. and Rumiantsev, S. V., 1995, Extreme Methods for Solving Ill-Posed Problems with Applications to Inverse Heat Transfer Problems, Springer Verlag.
- Beck, J. V. and Arnold, K. J., 1977, Parameter Estimation in Engineering and Science, Wisley, New York,.
- Blackwell, B. F., Dowding, K. J. and Cochran, 1999, Development and Implementation of Sensitivity Coefficient Equations for The Conduction Problems, Numerical Heat Transfer, Part 3, Vol. 36, pp. 15-32.
- Cotta, R. M., 1993, Integral Transforms in Computational Heat and Fluid Flow, CRC Press, Inc.
- Dantas, L.B., Orlande, H.R.B. and Cotta, R.M, 2002, Estimation of Dimensionless Parameters of Luikov's System for Heat and Mass Transfer in Capillary Porous Media, International Journal of Thermal Sciences, Vol. 41, pp. 217-227.
- Dantas, L.B., Orlande, H.R.B. and Cotta, R.M, 2003, An Inverse Problem of Parameter Estimation for Heat and Mass Transfer in Capillary Porous Media, International Journal of Heat and Mass Trnasfer, Vol. 46, pp. 1587-1598.
- Dietl, C., Winter, E.R.F. and Viskanta, R., 1998, An Efficient Simulation of the Heat and Mass Transfer Process During Drying of Capillary Porous, Higroscopic Material, International Journal of Heat and Mass Transfer, Vol. 4, pp. 3611-3625.
- Dolinskiy, A.A., Dorfman, A.Sh. and Davydenko, B.V., 1991, Conjugate Heat and Mass Transfer in Continuous Process of Convective Drying, International Journal of Heat and Mass Transfer, Vol. 34, pp. 2883-2889.
- Dowding, K.J., Blackwell, B.F. and Cochan, R.J., 1999, Applications of Sensitivity Coefficients for Heat Conduction Problems, Numerical Heat Transfer, Part B, Vol. 36, pp. 33-55.
- Emery, A. F., Fadale, T. D. and Nenarokomov, A. V., 1993, Optimal Sensor Location Considering Parameter Variability, 1<sup>st</sup> International Conference on Inverse Problems in Engineering Theory and Practice, pp. 361-368, Daytona, USA.
- Flach, G. P. and Özisik, M. N., 1989, Inverse Heat Conduction Problem of Simultaneously Estimating Spatially Varying Thermal Conductivity and Heat Capacity per Unit Volume, Numer. Heat Transfer, Vol. 16, pp. 249-266.
  Collent, A. P., 1987, Nonlinear Statistical Models, Wiley, New York.

Gallant, A. R., 1987, Nonlinear Statistical Models, Wiley, New York.

Huang, C. H. and Özisik, M. N., 1990, A Direct Integration Approach for Simultaneously Estimating Spatially Varying Thermal Conductivity and Heat Capacity, Int. J. Heat and Fluid Flow, Vol. 11, pp. 262-268.

- Huang, C. H. and Yeh, C. Y., 2002, An Inverse Problem in Simultaneous Estimating the Biot Number of Heat and Moisture Transfer for a Porous Material, International Journal of Heat and Mass Transfer, Vol. 45, pp. 4643-4653.
- Lobo, P.D.C., Mikhailov, M.D. and Özisik M.N., 1987, On the Complex Eigenvalues of Luikov System of Equations, Drying Technology, v. 5, n. 2, pp. 273-286.
- Lugon Jr., J., Pinheiro, R.P.F., Vasconcellos, J.F.V. and Silva Neto, A.J., 2002, A Sensitivity Study Applied to the Problem of Simultaneous Heat and Mass Transfer Diffusion in a One-Dimensional Porous Media, XXV National Congress on Applied and Computational Mathematics, Nova Friburgo, Brazil (in Portuguese).
- Lugon Jr., J., Pinheiro, R.P.F., Vasconcellos, J.F.V. and Silva Neto, A.J., 2002a, Inverse Problem of Simultaneous Heat and Mass Transfer in One-Dimensional Porous Media, V Meeting on Computational Modelling, pp. 93-102, Nova Friburgo, Brazil (in Portuguese).
- Luikov, A.V. and Mikhailov, M.D, 1965, Theory of Energy and Mass Transfer, Pergamon Press, Oxford, England.
- Marquardt, D. W., 1963, An Algorithm for Least-squares Estimation of Nonlinear Parameters, J. Soc. Industr. Appl. Math., Vol. 11, pp. 431-441.
- Meric, R. A., 1998, Shape Design Sensitivity Analysis and Optimization for Nonlinear Heat and Eletric Conduction Problems, Numerical Heat Transfer, Part A, Vol. 34, pp. 185-203.
- Mikhailov, M.D. and Özisik M.N., 1984, Unified Analysis and Solution of Heat and Mass Diffusion, Jonh Wiley, New York.
- Mikhailov, M.D., 1969, Etude Theorique de la Propagation de la Chaleur et de L'humidite, Int. J. Heat & Mass Transfer, v. 12, 1015-1024.
- Murio, D. A., 1993, The Mollification Method and the Numerical Solution of Ill-Posed Problems, John Wiley & Sons, New York.
- Orlande, H.R.B., 2002, Parameter and Function Estimation Problems in Heat and Mass Transfer, 5<sup>th</sup> World Congress on Computational Mechanics, Mini-Symposium MS125 Computational Treatment of Inverse Problems in Mechanics, Vienna, Austria.
- Silva Neto, A.J., 2002, Explicit and Implicit Formulations for the Inverse Radiative Transfer Problems, 5<sup>th</sup> World Congress on Computational Mechanics, Mini-Symposium MS 125 Computational Treatment of Inverse Problems in Mechanics, Vienna, Austria.
- Silva Neto, A.J. and Moura Neto, F.D., 1999, Model Choosing Inverse Problems in Engineering, Lecture Notes, XXII Brazilian Congress on Applied and Computational Mathematics, Santos, Brazil.
- Silva Neto, A.J. and Soeiro, F.J.C.P., 2001, A Combination of Gradient Based and Global Optimization Methods for the Solution of Inverse Heat Transfer Problems, IPES-2001, Inverse Problems in Engineering Symposium, College Station, USA.
- Silva Neto, A.J. and Soeiro, F.J.C.P., 2003, Solution of Implicitly Formulated Inverse Heat Transfer Problems with Hybrid Methods, Mini-Symposium Inverse Problems from Thermal/Fluids and Solid Mechanics Applications 2<sup>nd</sup> MIT Conference on Computational Fluid and Solid Mechanics, Cambridge, USA.
- Taktak, R. Beck, J. V. and Scott, E. P., 1003, Optimal Experimental Design for Estimating Thermal Properties of Composite Materials, International Journal of Heat and Mass Transfer, Vo. 36, No 12, pp. 2977-2986.
- Thum, R. L., Barichello, L. B., Vilhena, M. T. and Cotta, R. M., 1998, Solution of Luikov's Problem with the Integral Transform (GITT) and Laplace Transform, VIII Brazilian Congress of Engineering and Thermal Sciences, Vol. I, pp. 43-46, Rio de Janeiro, Brazil, (in Portuguese).
- Tseng, A. A., Cheng, T. C. and Zhao, F. Z., 1995, Direct Sensitivity Coefficient Method for Solving Two-Dimensional Inverse Heat Conduction Problems by Finite-Element Scheme, Numerical Heat Transfer, Part B, Vol. 27, pp. 291-307.